Institute of Inorganic Chemistry SAS

Questionnaire

Summary of the main activities of a research institute
of the Slovak Academy of Sciences

Period: January 1, 2016 - December 31, 2021

June 30, 2022, Bratislava

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doc. Ing. Miroslav Boča, DrSc.
Director IIC SAS

Contents

1. Basic information on the institute:

1.1. Legal name and address

Institute of Inorganic Chemistry (IIC SAS)
Slovak Academy of Sciences
Dúbravská cesta 9
SK-845 36 Bratislava
Slovak Republic

1.2. URL of the institute web site

http://www.uach.sav.sk/

1.3. Executive body of the institute and its composition

Directoriat	Name	Year of birth	Years in the position, from - to
Director	doc. Ing. Miroslav Boča, DrSc.	1973	2013 - present
Deputy director	doc. Ing. Miroslav Hnatko, PhD.	1973	2013 - present
Scientific secretary	doc. Ing. Zoltám Lenčéš, PhD.	1965	2014 - present

1.4. Head of the Scientific Board

RNDr. Jana Madejová, DrSc. - since 29.4.2014

1.4.1 Composition of the International Advisory Board

- Ing. Kamil Lang, CSc., DSc. (Institute of Inorganic Chemistry of the Czech Academy of Sciences, Husinec-Řež, Czech Republic)
- prof. Ralf Riedel Dr.h.c. (Department of Materials and Geosciences, Technische Universität Darmstadt, Germany)
- prof. Kenneth Ruud (University of Tromsø – The Arctic University of Norway)
- Dr. Mathieu Allix (CNRS, Orléans – Laboratoire CEMHTI, France)
- prof. RNDr. Karel Maca, Dr. (Institute of Materials Science and Engineering, Brno University of Technology, Czech Republic)

1.5. Basic information on the research personnel

1.5.1. Fulltime equivalent work capacity of all employees (FTE all), FTE of employees with university degrees engaged in research projects (FTE researchers)

2016		2017		2018		2019		2020		2021		2016-2021	
FTE all	FTE researchers	FTE all	FTE researchers	FTE all	FTE researchers	FTE all	FTE researchers	FTE all	FTE researchers	FTE all	FTE researchers	average FTE all per year	average FTE researchers per year
59.43	45.88	60.00	44.34	62.20	46.01	57.38	40.71	57.46	40.18	59.49	43.51	**59.33**	**43.44**

1.5.2. If applicable, add also a short information on the merger of the institute in the evaluation period. You can also add rows in the above table corresponding to the founding institutes

1.6. Basic information on the funding of the institute

1.6.1. Institutional salary budget, other salary budget[1], non-salary budget[2]

Salary budget	2016	2017	2018	2019	2020	2021	average
Institutional salary budget *[millions of EUR]*	0.959	1.101	1.113	1.210	1.347	1.379	**1.185**
Other salary budget *[millions of EUR]*	0.179	0.166	0.267	0.250	0.262	0.268	**0.232**
Total salary budget *[millions of EUR]*	1.138	1.267	1.380	1.460	1.609	1.647	**1.417**
Non-salary budget *[millions of EUR]*	0.484	0.578	0.591	0.630	0.573	0.675	**0.589**

1.7. Mission Statement of the Institute as presented in the Foundation Charter indicating the years when it was adopted and revised

The Foundation Charter from 27.8.2008 states:

1. The Institute of Inorganic Chemistry (IIC) is focused on basic research in the area of inorganic and bio-inorganic systems oriented to optimization and development of new materials and technological processes in the following branches of science:
   - Inorganic chemistry
   - Physical chemistry
   - Materials chemistry
   - Inorganic technologies and materials
   - Theoretical chemistry
   - Nanotechnology

[1] Salary budget originating outside the regular budgetary resources of the organization, e.g. from the project funding.
[2] Includes Goods and Services and PhD fellowships

2. The Institute performs scientific education pursuant to generally binding legal regulations.
3. The Institute provides consulting and expertise services related to the main activity of the Institute.
4. The main subjects of the research are the following:
   - Relations between composition, properties and structure of inorganic substances, mainly advanced ceramic materials, molten salt systems and hydrosilicates.
   - Thermodynamics of multicomponent systems.
   - Features and chemical reactions of inorganic systems, including interfaces of phases.
   - Development and application of theoretical and experimental methods for the determination of the structure and properties of matter.

Although all statements in the Foundation Charter are still valid, the mission of the Institute has been continuously developing since 2008. The Institute systematically incorporates additional research subjects in related scientific areas in response to current scientific and societal challenges. More details are given in the next chapter.

1.8. Summary of R&D activity pursued by the institute during the evaluation period in both national and international contexts. Describe the scientific importance and societal impact of each important result/discovery. Explain on general level – the information should be understandable for a non-specialist (recommended 5 pages, max. 10 pages for larger institutes with more than 50 average FTE researchers per year as per Table 1.5.1.)

The R&D activities of the Institute are affected by many factors, including:

- The context of the research topics.
- Human resources – the composition of research teams (young researchers, senior researchers or leading authorities), the presence of technicians, and interest in specific topics by PhD students. Also, exchange of researchers and international cooperation play an important role.
- Financial sources – domestic grants (APVV, VEGA, structural funds) and international grants (bilateral or multilateral) including H2020 grant schemes.
- State research strategy/support and legislative background.
- All these issues should be properly balanced in order to provide an appropriate basis for effective scientific activities and competition. Some comments on this will be provided below (chapter 2.1.8 and 2.9.). In the following part we will provide a concise evaluation of the R&D activities of particular departments.

Department of Ceramics

The primary interest of the Department of Ceramics is to understand the relations between the microstructural and mechanical properties of oxide/non-oxide ceramic nano/micro-composites and ceramic/metal composites. Microstructural design of new types of composites with excellent functional (e.g. high thermal and/or electrical conductivity) and mechanical properties, luminescent materials, corrosion and oxidation resistant materials, etc. is the primary area of research. The experimental research is combined with theoretical ab-initio approaches for the design and explanation of engineering and functional properties of ceramics.
Part of the research is focused on the development and joining of **ultra-high temperature ceramic matrix composites** for extreme applications, such as in the aerospace and nuclear industries [1]. The improved high temperature properties are obtained by the microstructural design of the materials and the use of appropriate additives. The application potential of these materials is significantly enhanced by the development of new, reliable, and user-friendly joining approaches.

The research activities are also focused on the **development of functionally-graded bioactive silicon nitride by surface thermal treatment using an oxyacetylene flame** [3]. The heat treatment forms a porous bioactive layer on the surface of the material, enabling human cell ingrowth. Such materials are desirable for their potential use in human bone replacements.
The Department has also worked on the **preparation and photocatalytic activity of TiO_2 nanotube arrays prepared on a transparent spinel substrate** [4]. The nanotubes, prepared by anodic oxidation of titanium, showed good photocatalytic activity with remarkable removal of pollutants (model pollutants rhodamine B and bisphenol A) from water.
The **preparation and mechanical and functional properties of ceramic composites with carbon nanostructures,** including carbon nanotubes (CNTs), graphene nanoplatelets (GNPs) and graphene oxide (GO) [5-8], have been studied. The highest electrical conductivity (11800 S/m) was obtained for SiC ceramics containing 10 % GNPs, while the highest thermal conductivity (~240 W/m·K) was obtained for SiC samples containing 5 % GNPs.
Another branch of research is oriented towards the design of new types of refractories containing zirconium oxycarbide or oxynitride ceramic phases. This area of research is closely associated with collaboration with industry (RHI Magnesita GmbH, Austria).

1. TATARKO, Peter** - VALENZA, Fabrizio - ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Design of Lu2O3-reinforced Cf/SiC-ZrB2-ZrC ultra-high temperature ceramic matrix composites: Wetting and interfacial reactivity by ZrSi2 based alloys. In Journal of the European Ceramic Society, 2021, vol. 41, p. 3051-3060. (2020: 5.302 - IF, Q1 - JCR, CCC). 10.1016/j.jeurceramsoc.2020.05.055
2. KIM, Young-Wook - KULTAYEVA, Shynar - SEDLÁČEK, Jaroslav - HANZEL, Ondrej - TATARKO, Peter - LENČÉŠ, Zoltán - ŠAJGALÍK, Pavol**. Thermal and electrical properties of additive-free rapidly hot-pressed SiC ceramics. In Journal of the European Ceramic Society, 2020, vol. 40, no. 2, p. 234-240. (2019: 4.495 - IF, Q1 - JCR, CCC). 10.1016/j.jeurceramsoc.2019.10.015
3. HNATKO, Miroslav** - HIČÁK, Michal - LABUDOVÁ, Martina - GALUSKOVÁ, Dagmar - SEDLÁČEK, Jaroslav - LENČÉŠ, Zoltán - ŠAJGALÍK, Pavol. Bioactive silicon nitride by surface thermal treatment. In Journal of the European Ceramic Society, 2020, vol. 41, no. 54, p. 1848-1858. (2019: 4.495 - IF, Q1 - JCR, CCC) 10.1016/j.jeurceramsoc.2019.12.053
4. PETRISKOVÁ, Patrícia - MONFORT, O. - SATRAPINSKYY, Leonid - DOBROČKA, Edmund - PLECENIK, T. - PLESCH, Gustáv - PAPŠÍK, Roman - BERMEJO, Raúl - LENČÉŠ, Zoltán**. Preparation and photocatalytic activity of TiO2 nanotube arrays prepared on transparent spinel substrate. In Ceramics International, 2021, vol. 47, no. 9, p. 12970-12980. (2020: 4.527 - IF, Q1 - JCR, CCC) 10.1016/j.ceramint.2021.01.160
5. HANZEL, Ondrej - LOFAJ, František - SEDLÁČEK, Jaroslav - KABÁTOVÁ, Margita - KAŠIAROVÁ, Monika - ŠAJGALÍK, Pavol. Mechanical and tribological properties of alumina-MWCNTs composites sintered by rapid hot-pressing. In Journal of the European Ceramic Society, 2017, vol. 37, no. 15, p. 4821-4831. (2016: 3.454 - IF, Q1 - JCR, CCC). 10.1016/j.jeurceramsoc.2017.05.047
6. HANZEL, Ondrej - SEDLÁK, Richard - SEDLÁČEK, Jaroslav - BIZOVSKÁ, Valéria - BYSTRICKÝ, Roman - GIRMAN, Vladimír - KOVALČÍKOVÁ, Alexandra - DUSZA, Ján - ŠAJGALÍK, Pavol. Anisotropy of functional properties of SiC composites with GNPs, GO and in-situ formed graphene. In Journal of the European Ceramic Society, 2017, vol. 37, p. 3731-3739. (2016: 3.454 - IF, Q1 - JCR, CCC) 10.1016/j.jeurceramsoc.2017.03.060
7. HANZEL, Ondrej** - SINGH, Meinam Annebushan - MARLA, Deepak - SEDLÁK, Richard - ŠAJGALÍK, Pavol. Wire electrical discharge machinable SiC with GNPs and GO as the electrically conducting filler. In Journal of the European Ceramic Society, 2019, vol. 39, no. 8, p. 2626-2633. (2018: 4.029 - IF, Q1 - JCR, 1.219 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jeurceramsoc.2019.03.012
8. HANZEL, Ondrej** - LENČÉŠ, Zoltán - KIM, Young-Wook - FEDOR, Ján - ŠAJGALÍK, Pavol. Highly electrically and thermally conductive silicon carbide-graphene composites with yttria and scandia additives. In Journal of the European Ceramic Society, 2020, vol. 40, no. 2, p. 241-250. (2019: 4.495 - IF, Q1 - JCR, CCC). 10.1016/j.jeurceramsoc.2019.10.001

Department of Hydrosilicates

The research activities of the Department are focused on layered hydrosilicates, which are natural or synthetic nanomaterials with extensive industrial use. The department's research has covered the latest scientific trends in the field, whether in the preparation of new functional nanomaterials or in the use of advanced experimental methods for detailed characterization and monitoring of their properties. In general, the research in this period has focused on two main areas: firstly, modification of smectites and their synthetic analogues using surface-active molecules to develop inorganic-organic composite materials, to be used for preparation of nanocomposites with polymer matrices or adsorbents which are very effective in the environment protection; and secondly, development of hybrid materials with organic dyes. Productive collaboration with various national and foreign institutions has expanded the scope of the research to several other fields, such as the synthesis of porous materials for catalysis and for adsorption of pharmaceuticals. The strength of the department is the methodological background of the researchers in the area of basic characterization of layered hydrosilicates, IR spectroscopy, UV-Vis and fluorescence spectroscopy. Based on the analysis of the results using these methods, original interpretations of the phenomena in the studied systems were drawn up.

Hybrid systems based on layered silicates and organic dyes, in forms including colloids, solid films and powders, were investigated, mainly by methods of spectroscopies in the visible region, in particular by absorption and fluorescence spectroscopy. Organic dyes were selected based on their

chemical properties and photoactivity. The layered silicates are rather inert and photochemically-inactive substrates, which, however, had very strong secondary effects on the properties of the adsorbed dye molecules. The materials were studied from various different aspects, from the mechanisms associated with their formation to the functionalities related to their photochemical parameters. By a suitable choice of the layered silicate and the chemical modification in the hybrid system, it was possible to stabilize the dye molecules, to tune their optical properties, and to increase their photoactivity. It is worth mentioning some interesting properties of these systems, such as optical anisotropy, transfer of excitation energy between adsorbed dye molecules, adsorption-induced luminescence, metachromasy and molecular aggregation, photosensitizing and photodisinfection. Polymer-composite surfaces functionalized with such hybrid particles exhibited anti-biofilm properties.

1. BOHÁČ, Peter - CZÍMEROVÁ, Adriana - BUJDÁK, Juraj. Enhanced luminescence of 3,3'-diethyl-2,2'-thiacyanine cations adsorbed on saponite particles. In Applied Clay Science, 2016, vol. 127-128, p. 64-69. (2.586 - IF2015).
2. ŠIMONOVÁ, T.** - MÉSZÁROS, R. - SEBECHLEBSKÁ, T. - BUJDÁK, J.** Non-Arrhenius kinetics and slowed-diffusion mechanism of molecular aggregation of a rhodamine dye on colloidal particles. In Physical Chemistry Chemical Physics, 2021, vol. 23, no. 32, p. 17177-17185. (2020: 3.676 - IF, Q1 - JCR, 1.053 - SJR, Q1 - SJR). ISSN 1463-9076.
3. BARLOG, M.** - PÁLKOVÁ, H. - BUJDÁK, J. Luminescence of a laser dye in organically-modified layered silicate pigments. In Dyes and Pigments, 2021, vol. 191, p. 109380-1-109380-11. (2020: 4.889 - IF, Q1).
4. BELUŠÁKOVÁ, Silvia – MARTÍNEZ-MARTÍNEZ, V. – LOPEZ ARBELOA, I. – BUJDÁK, Juraj. Resonance energy transfer between dye molecules in colloids of a layered silicate. The effect of dye surface concentration. In Journal of Physical Chemistry C, 2017, vol. 121, p. 8300-8309. (4.536 – IF2016). ISSN 1932-7447. ADCA

New results concerning the **conformation of alkylammonium surfactants in clay mineral interlayers** represent a significant contribution to the development of organoclays with tailored structural characteristics, which is of great importance for their application as adsorbents for pollutants or fillers for clay-based polymer nanocomposites. The effect of the alkyl chain length, head-group structure ($-N(CH_3)_3$ *vs*. $-NH_3$), and temperature on the arrangement of surfactants was investigated in detail by XRD, near-IR and ^{13}C NMR spectroscopy. On increasing number and length of the alkyl chains a number of disordered *gauche* conformers decreased and ordered all-*trans* increased. Higher abundance of *gauche* conformers for C*X*$-NH_3$ than for C*X*$-N(CH_3)_3$ surfactants was found for shorter alkyl chains (*X*=6 - 10); the effect of the head-group was reduced for the longer chains with 12 – 18 carbons. With increasing temperature the alkyl tails adopted a more disordered, liquid-like structure. On contrary, the samples cooled to the temperature of liquid nitrogen showed the dominance of well-ordered all-*trans* conformer characteristic of a crystalline-like state [5-7].

5. BIZOVSKÁ, Valéria - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana. Montmorillonite modified with unconventional surfactants from the series of octylammonium-based cations: Structural characterization and hydration properties. In Applied Clay Science, 2018, vol. 158, p. 102-112. (3.641 - IF2017).
6. SLANÝ, Michal** - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana. Structural characterization of organo-montmorillonites prepared from a series of primary alkylamines salts: Mid-IR and near-IR study. In Applied Clay Science, 2019, vol. 176, p. 11-20. (2018: 3.890 - IF, Q1 – JCR, CCC).
7. MADEJOVÁ, Jana** - JANKOVIČ, Ľuboš - SLANÝ, Michal - HRONSKÝ, Viktor. Conformation heterogeneity of alkylammonium surfactants self-assembled on montmorillonite: Effect of head-group structure and temperature. In Applied Surface Science, 2020, vol. 503, p. 144125-1-144125-11. (2019: 6.182 - IF, Q1 – JCR, CCC). 10.1016/j.apsusc.2019.144125

Department of Molten Systems

The research interests of the department comprise the investigation of physico-chemical (phase equilibria, density, electric conductivity, viscosity, and surface tension), electro-chemical (various types of voltammetry, chronoamperometry, chronopotentiometry, electrochemical impedance spectroscopy), thermo-chemical (DTA, DSC, c_p), spectral (NMR, XPS, XRF, IR) and diffraction (X-ray and neutron powder diffraction and single-crystal analysis) properties of predominantly fluoride salts. The ultimate goal is to find the relationship between the physico-chemical behaviour of the molten systems and their composition and structure, using thermodynamic models as well as quantum-mechanical simulations. The research focuses mainly on **fluoride systems based on Al, Mg, Zr, Sc, Ta, Nb, and systems based on lanthanides** (all with additions of a variety of other compounds). The applied research of the department is mainly connected with optimization of the conditions of the electrolytic production of primary aluminium, as well as other electrolytically-deposited metals, but the subjects of our applied research are not limited only to electrometallurgy. An important part of the research is the study of corrosion of construction materials in melts, the investigation of molten systems suitable for energy storage, and the synthesis of interesting compounds from inorganic melts, e.g. ternary fluorides for photonic and electronic applications. The

variety of research methodologies used, research topics, and interests in applied research enables the department to be involved in various national and international projects and collaborations with academia, as well as in applied research for foreign and domestic industrial partners. The extraordinary position of the department in the field can be further demonstrated by the exceptional infrastructure developed at the department. We are the only lab in the world with special, non-commercial equipment for measuring all of the main physico-chemical properties in one place. Our data are often used as reference data for other labs.

Critical elements: To address the growing concern regarding valuable raw materials for the EU economy, the European Commission launched the European Raw Materials Initiative in order to boost resource efficiency and promote recycling. Systematic research on various fluorides of lanthanide elements (La, Nd, Sm, Gd) and other critical materials like magnesium, silicon, and niobium is the primary focus of the department's research activities. Various aspects of the studied systems were experimentally analysed, such as the solubility of the fluorides and oxides of critical elements in molten fluorides, and their basic physico/thermo/electro-chemical properties in order to provide necessary data for practical industrial applications. The spectral and diffraction characterization was also a research focus in order to understand the formation and transformation of particular phases present in the system. All these activities contribute to the effort of economically-effective and environmentally-friendly recovery and recycling of the highly-demanded critical elements and materials. This research was mostly done in cooperation with our partners from Europe, USA, and China.

1. ŠIMKO F** – RAKHMATULLIN, Aydar – FLORIAN, Pierre – KONTRÍK, Martin – KORENKO, Michal – NETRIOVÁ, Zuzana – DANIELIK, Vladimír – BESSADA, Catherine. (Oxo)(fluoro)-aluminates in KF-Al2O3 system: thermal stability and structural correlation. In Inorganic Chemistry, 2017, vol. 56, no. 21, p. 13349-13359. (2016: 4.857 – IF). https://doi.org/10.1021/acs.inorgchem.7b02105
2. KORENKO, Michal** – LARSON, Carol – BLOOD, K. – PALUMBO, Robert – NUDEHI, S. – DIVER, R. – BLOOD, D. – ŠIMKO, František – VENSTROM, Luke J. Technical and economic evaluation of a solar thermal MgO electrolysis process for magnesium production. In Energy, 2017, vol. 135, p. 182-194. (2016: 4.520 – IF). 10.1016/j.energy.2017.06.044
3. KUBÍKOVÁ, Blanka - MLYNÁRIKOVÁ, Jarmila - BENEŠ, Ondřej - MIKŠÍKOVÁ, Eva - PRIŠČÁK, Jozef - TOSOLIN, Alberto - BOČA, Miroslav**. Physico-chemical properties of the system (LiF-NaF)eut-LaF3 - Phase equilibria, density and volume properties, electrical conductivity and surface tension. In Journal of Molecular Liquids, 2018, vol. 268, p. 754-761. (2017: 4.513 - IF, Q1 - JCR, 0.849 - SJR, Q1 - SJR). 10.1016/j.molliq.2018.07.114
4. KORENKO, Michal** – ŠIMKO, František – MLYNÁRIKOVÁ, Jarmila – LARSON, Carol – MIKŠÍKOVÁ, Eva – PRIŠČÁK, Jozef – AMBROVÁ, Marta – PALUMBO, Robert. Physico-chemical properties of $(MgF_2\text{-}CaF_2\text{-}(LiF))_{eut}$-MgO system as a molten electrolyte for Mg electrowinning. In Journal of Molecular Liquids, 2019, vol. 275, p. 535-543. (2018: 4.561 – IF). 10.1016/j.molliq.2018.11.066
5. BOČA, Miroslav** - MLYNÁRIKOVÁ, Jarmila - MACKOVÁ, Iveta - JANIČKOVIČ, Dušan - CZÍMEROVÁ, Adriana - SHI, Zhongning. Diffraction and luminescence analysis of extremely rapidly cooled molten system $(LiF\text{-}CaF_2)$(eut)-xLnF(3) (Ln=Sm and Gd). In Transactions of Nonferrous Metals Society of China, 2021, vol. 31, no. 4, p. 1151-1164. (2020: 2.917 - IF, Q1 - JCR, 0.744 - SJR, Q1 - SJR). 10.1016/S1003-6326(21)65568-1

Department of Theoretical Chemistry

One of the main directions of the Department of Theoretical Chemistry is the development of **new, efficient methods for relativistic calculations and interpretation of the spectroscopic properties** of heavy-element compounds. In order to be available to practical chemists, the new methods are implemented in the ReSpect program founded also by members of Department (http://respectprogram.org/). This program allows one to employ a variety of state-of-the art computational tools, including the calculation of linear and non-linear optical properties, by efficiently solving the time-dependent Dirac equation [1]. The philosophy and functionality of the code, including its newest features, is described in ref [2], which serves as the introduction to the ReSpect program for a wide international audience of potential users.

Newly-developed quantum-chemical tools for the analysis and interpretation on NMR parameters helped to identify the rules governing relativistic spin−orbit heavy-neighbour-atom effects on NMR shifts. In particular, spin-orbit effects on NMR ligand shieldings in transition metal complexes of Pt(II), Au(I), Au(III), and Hg(II) were studied [3]. The results suggested that the principles identified in this work have general validity across the periodic table. This was elaborated and general rules for the observed trends were formulated in ref [4]. The discovered trends were then further explained in a comprehensive review [5]. The review provides guidelines for helping NMR spectroscopists and computational chemists to estimate the ranges of the NMR shifts for unknown compounds, identify intermediates in catalytic and other processes, analyse conformational aspects and intermolecular interactions, and predict trends in series of compounds throughout the Periodic Table. This improvement in our understanding additionally opens up broader possibilities in research into substances containing heavy elements, such as the design of new anti-cancer drugs or the study of the spread of leaked nuclear waste into the environment.

In addition to work on our in-house code ReSpect we also contribute to other quantum chemical codes to made our methods broadly available to the research community. In the highly-popular periodic DFT code VASP we have implemented a physically-sound and computationally-affordable model for describing long-range dispersion interactions within DFT [6]. We were the first to adapt the accurate many-body dispersion scheme for use with periodic systems, thus enabling its use in simulation protocols such as structural relaxations or molecular dynamics.
Within our department we also pay special attention to the application of quantum chemical methodologies in important chemical applications. An important research direction is the study of the structural stability of proposed new materials by applying *ab initio* DFT methods to the structure of clays, e.g. beidellite modified by a series of organic surfactants (alkylphosphonium cations). Stable hybrid forms of these advanced materials (organoclays) are crucial for their use as adsorbents for remediation of ground/wastewater contaminated by, e.g., drugs or pesticides. The calculated intercalation energies of the studied systems – taken as a measure of their structural stabilities – grew with the length of the alkyl chain of the organic surfactant [7]. Another theoretical study of the mechanical properties of a clay mineral modified with methoxy-containing compounds showed improved exfoliating properties of this material, which are desirable for the synthesis of new polymer nanocomposites. Such a modification increases the grafted kaolinite's exfoliation properties by ca. +15% compared to those of pure kaolinite [8]. Another example of the application of quantum chemical methodologies is our study of the indirect spin-spin coupling between two hydrogen atoms formally separated by up to 18 covalent bonds. This was observed for the first time by NMR experiments on a model helical molecule [9]. The direct distance between the interacting protons was about 3 Å. It was shown that this interaction can provide essential information about the molecular conformation in solution. The interaction pathways were visualized and analyzed by computational methods. The newly-discovered phenomenon was then explained on the basis of this analysis.

1. KONEČNÝ L – KÁDEK M – KOMOROVSKÝ S – MALKIN O – RUUD K – REPISKÝ M. Acceleration of relativistic electron dynamics by means of X2C transformation: Application to the calculation of nonlinear optical properties. Journal of Chemical Theory and Computation 2016, 12, p. 5823-5833. (IF2015: 5.301, Q1 – JCR, CCC) 10.1021/acs.jctc.6b00740
2. REPISKÝ M** – KOMOROVSKÝ S** – KÁDEK M – KONEČNÝ L – EKSTRÖM U – MALKIN E – KAUPP M – RUUD K – MALKIN O – MALKIN V. ReSpect: Relativistic spectroscopy DFT program package. Journal of Chemical Physics 2020, 152, p. 184101-1-36. (IF2019: 2.991, Q2 – JCR, CCC) 10.1063/5.0005094
3. NOVOTNÝ J – VÍCHA J – BORA P L – REPISKÝ M – STRAKA M – KOMOROVSKÝ S** – MAREK R**. Linking the character of the metal-ligand bond to the ligand NMR shielding in transition-metal complexes: NMR contributions from spin-orbit coupling. Journal of Chemical Theory and Computation 2017, 13, p. 3586-3601. (IF2016: 5.245, Q1 – JCR, CCC) 10.1021/acs.jctc.7b00444
4. VÍCHA J** – KOMOROVSKÝ S – REPISKÝ M – MAREK R – STRAKA M**. Relativistic spin-orbit heavy atom on the light atom NMR chemical shifts: General trends across the periodic table explained. Journal of Chemical Theory and Computation 2018, 14, p. 3025-3039. (IF2017: 5.399, Q1 – JCR, CCC) 10.1021/acs.jctc.8b00144
5. VÍCHA J – NOVOTNÝ J – KOMOROVSKÝ S – STRAKA M** – KAUPP M** – MAREK R**. Relativistic heavy-neighbor-atom effects on NMR shifts: Concepts and trends across the periodic table. Chemical Reviews 2020, 120, p. 7065-7103. (IF2019: 52.758, Q1 – JCR, CCC) 10.1021/acs.chemrev.9b00785
6. BUČKO T – LEBÈGUE S – GOULD T – ÁNGYÁN J G. Many-body dispersion corrections for periodic systems: an efficient reciprocal space implementation. Journal of Physics: Condensed Matter 2016, 28, p. 045201-1-13. (IF2015: 2.209, Q2 – JCR, CCC) 10.1088/0953-8984/28/4/045201
7. JANKOVIČ Ľ** – ŠKORŇA P – MORENO RODRÍGUEZ D – SCHOLTZOVÁ E – TUNEGA D. Preparation, characterization and adsorption properties of tetraalkylphosphonium organobeidellites. Applied Clay Science 2021, 204, p. 105989-1-10. (IF2020: 5.467, Q1 – JCR, CCC). 10.1016/j.clay.2021.105989
8. SCHOLTZOVÁ E** – TUNEGA D**. Prediction of mechanical properties of grafted kaolinite – A DFT study. Applied Clay Science 2020, 193, p. 105692-1-7. (IF2019: 4.605, Q1 – JCR, CCC) 10.1016/j.clay.2020.105692
9. DRAČÍNSKÝ M** – BUCHTA M – BUDĚŠÍNSKÝ M – VACEK-CHOCHOLOUŠOVÁ J – STARÁ I G – STARÝ I – MALKIN O**. Dihydrogen contacts observed by through-space indirect NMR coupling. Chemical Science 2018, 9, p. 7437-7446. (IF2017: 9.063, Q1 – JCR, CCC) 10.1039/c8sc02859a

Joint Glass Centre (Vitrum Laugaricio, acr. VILA)

The VILA Department, as a joint laboratory of the IIC SAS, Alexander Dubček University of Trenčín, and Faculty of Chemical and Food Technology Slovak University of Technology, focuses its activities on the study of fundamental relations between the composition, structure, and physical properties of inorganic non-metallic materials, with a special focus on **oxide glasses and glass-forming melts**. The main topics include volumetric studies, structural and enthalpy relaxation processes in silicate glasses, thermodynamic modelling and molecular dynamic simulations of the structure of glasses, study of processes during glass batch melting, and the electrochemistry of glasses and glass melts. The research area also involves research related to vitrification and immobilization of radioactive waste and the study of glass-fibre based insulation for nuclear power-plants. The VILA Department also deals with innovative methods of glass production (e.g. flame synthesis) which have opened

the way to the preparation of unique materials, for example porous bioactive glass microspheres for drug delivery or optically-active glass microspheres [1-6].
Strong ties exist with local industry, as demonstrated by the numerous research activities for regional glass producers (most notably, development of new types of utility glasses with high corrosion resistance for RONA j.s.c. Lednické Rovne, and optimization of glass melting and elimination of foam formation for Johns Manville Slovakia, Trnava).

1. HALADEJOVÁ, Katarína - PRNOVÁ, Anna - KLEMENT, Róbert - TUAN, Wei-Hsing - SHIH, S. J. - GALUSEK, Dušan. Aluminate glass based phosphors for LED applications. In Journal of the European Ceramic Society, 2016, vol. 36, no. 12, p. 2969-2973. (2.933 - IF2015). https://doi.org/ 10.1016/j.jeurceramsoc.2015.11.027
2. CHROMČÍKOVÁ, Mária - VOKELOVÁ, Jana - MICHÁLKOVÁ, Jaroslava - LIŠKA, Marek - MACHÁČEK, Jan - GEDEON, Ondrej - SOLTÉSZ, Vojtech. Chemical durability of gamma-irradiated glass fibrous insulation. In Nuclear Technology, 2016, vol. 193, no. 2, p. 297-305. (0.623 - IF2015). https://doi.org/ 10.13182/NT15-22
3. KRAXNER, Jozef - MICHÁLEK, Martin - ROMERO, Acacio Rincon - ELSAYED, Hamada - BERNARDO, Enrico - BOCCACCINI, Aldo - GALUSEK, Dušan. Porous bioactive glass microspheres prepared by flame synthesis process. In Materials Letters, 2019, vol. 256, p. 126625-1-126625-4. (2018: 3.019 - IF, Q2 - JCR). https://doi.org/10.1016/j.matlet.2019.126625
4. CHROMČÍKOVÁ, Mária – HRUŠKA, Branislav – SVOBODA, Roman – LIŠKA, Marek – NOWICKA, Aleksandra – BRUNEEL, Els – De BUYSSER, Klaartje. Identification of surface active components in glass forming melts by thermodynamic model. In Journal of Non-Crystalline Solids 551 (2021) 120415. 10.1016/j.jnoncrysol.2020.120415
5. PRNOVÁ, Anna - KLEMENT, Róbert - BODIŠOVÁ, Katarína - VALÚCHOVÁ, Jana - GALUSEK, Dušan - BRUNEEL, Els - VAN DRIESSCHE, Isabelle. Thermal behaviour of yttrium aluminate glasses studied by DSC, high-temperature X-ray diffraction, SEM and SEM–EDS. In Journal of Thermal Analysis and Calorimetry 128 (2017) 1407-1415. IF=1.953 doi.org/10.1007/s10973-016-6078-2
6. MICHÁLKOVÁ, Monika - KRAXNER, Jozef - PARCHOVIANSKÝ, Milan - KLEMENT, Róbert - POUCHLÝ, Václav - MACA, Karel - GALUSEK, Dušan. Viscous flow spark plasma sintering of glass microspheres with YAG composition and high tendency to crystallization. In Journal of the European Ceramic Society, 41 (2021) 1537–1542. (4.495 – IF2019). ISSN 09552219. 10.1016/j.jeurceramsoc.2020.10.015

The second field of research in the VILA Department is the study of the **processing, microstructure, and properties of transparent polycrystalline oxide ceramic materials** such as alumina, yttria or magnesium aluminate spinel with excellent optical properties. Research also focuses on developing a new generation of luminescent optoelectronics materials with high efficiency, low-cost production and adjustable/adaptable luminescent properties [7-8].

7. DRDLÍKOVÁ, Katarína - KLEMENT, Róbert - DRDLÍK, Daniel - SPUSTA, Tomáš - GALUSEK, Dušan - MACA, Karol. Luminescent Er3+-doped transparent alumina ceramics. In Journal of European Ceramics Society 37 (2017) 2695-2703. IF: 3.411. 10.1016/j.jeurceramsoc.2017.02.017
8. TALIMIAN, Ali - POUCHLÝ, Václav - EL-MAGHRABY, Hesham F. M. Aldelrehim - MACA, Karel - GALUSEK, Dušan. Transparent magnesium aluminate spinel: Effect of critical temperature in two-stage spark plasma sintering. In Journal of the European Ceramic Society, 2020, vol. 40, no. 6, p. 2417-2425. (2019: 4.495 - IF, Q1 - JCR, 1.164 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jeurceramsoc.2020.02.012

2. Partial indicators of main activities:

2.1. Research output

2.1.1. Principal types of research output of the institute: basic research/applied research, international/regional (in percentage)

In the assessed period, the Institute was mainly oriented towards its fundamental research (as stated in the Foundation Charter). In addition to this primary activity, there was a significant effort to initialize, develop or expand activities involving applied research in areas which attract interest from the broader scientific community. However, the success of such activities depends on the interest of industrial partners. The ratio of basic to applied research thus can be estimated as 3:1 (i.e. 25 % applied research).

The research activities of the Institute are oriented mostly to the international research area. This is determined by the Institute's focus on scientific activities that cannot be effectively carried out without international cooperation. Of course, even in collaborative work, it is common for the regional research teams to specialise in different research topics related to the overall subject of the project. The ratio of international to regional research can be estimated as ca. **9:1 (*i.e.* 10 % regional research)**.

The level of co-operation with industry is expected to increase in the next few years. Nevertheless, we shall continue to strive for excellence in the fundamental research which forms the necessary basis for advanced applied research. To achieve this aim, it is necessary to have high quality human resources. Involvement in international research consortia and projects should create a framework for this effort. All these activities should lead to an increase in the quality of research performed at the Institute.

2.1.2 List of selected publications documenting the most important results of basic research. The total number of publications should not exceed the number of average FTE researchers per year. The principal research outputs (max. 10% of the total number of selected publications, including Digital Object Identifier – DOI if available) should be underlined. Authors from the evaluated organizations should be underlined.

The following selection of publications has been chosen to cover as much of the diversity of the research conducted by the Institute as possible. Consequently, it is not simply a list of papers published just in the highest-impact journals, but rather a list of the most important papers within individual fields of interest to show the diversity and complementarity in particular topics and cooperation.

Department of Ceramics

1. TATARKO, Peter** - VALENZA, Fabrizio - ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Design of Lu2O3-reinforced Cf/SiC-ZrB2-ZrC ultra-high temperature ceramic matrix composites: Wetting and interfacial reactivity by ZrSi2 based alloys. In Journal of the European Ceramic Society, 2021, vol. 41, p. 3051-3060. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jeurceramsoc.2020.05.055
2. ÜNSAL, Hakan - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - TATARKOVÁ, Monika - DLOUHÝ, Ivo - TATARKO, Peter**. In-situ graphene platelets formation and its suppression during reactive spark plasma sintering of boron carbide/titanium diboride composites. In Journal of the European Ceramic Society, 2021, vol. 41, no. 13, p. 6281-6289. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jeurceramsoc.2021.06.053
3. HNATKO, Miroslav** - HIČÁK, Michal - LABUDOVÁ, Martina - GALUSKOVÁ, Dagmar - SEDLÁČEK, Jaroslav - LENČÉŠ, Zoltán - ŠAJGALÍK, Pavol. Bioactive silicon nitride by surface thermal treatment. In Journal of the European Ceramic Society, 2020, vol. 41, no. 54, p. 1848-1858. (2019: 4.495 - IF, Q1 - JCR, 1.164 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jeurceramsoc.2019.12.053

4. HNATKO, Miroslav - KAŠIAROVÁ, Monika - GALUSKOVÁ, Dagmar - BYSTRICKÝ, Roman - LENČÉŠ, Zoltán - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Corrosion of engineering ceramic materials by molten iron part I: Silicon nitride and SiAlON. In Corrosion Science, 2016, vol. 107, p. 76-84. (2015: 5.154 - IF, Q1 - JCR, 1.907 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.corsci.2016.02.021
5. HANZEL, Ondrej** - LENČÉŠ, Zoltán - KIM, Young-Wook - FEDOR, Ján - ŠAJGALÍK, Pavol. Highly electrically and thermally conductive silicon carbide-graphene composites with yttria and scandia additives. In Journal of the European Ceramic Society, 2020, vol. 40, no. 2, p. 241-250. (2019: 4.495 - IF, Q1 - JCR, 1.164 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jeurceramsoc.2019.10.001
6. ŠAJGALÍK, Pavol - SEDLÁČEK, Jaroslav - LENČÉŠ, Zoltán - DUSZA, Ján - LIN, Hua-Tay. Additive-free hot-pressed silicon carbide ceramics - A material with exceptional mechanical properties. In Journal of the European Ceramic Society, 2016, vol. 36, no. 6, p. 1333-1341. (2015: 2.933 - IF, Q1 - JCR, 1.135 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jeurceramsoc.2015.12.013
7. TATARKOVÁ, Monika** - TATARKO, Peter - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - DUSZA, Ján - ŠAJGALÍK, Pavol. Influence of hexagonal boron nitride nanosheets on phase transformation, microstructure evolution and mechanical properties of Si3N4 ceramics. In Journal of the European Ceramic Society, 2021, vol. 41, no. 10, p. 5115-5126. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jeurceramsoc.2021.01.057
8. PETRISKOVÁ, Patrícia - MONFORT, O. - SATRAPINSKYY, Leonid - DOBROČKA, Edmund - PLECENIK, T. - PLESCH, Gustáv - PAPŠÍK, Roman - BERMEJO, Raúl - LENČÉŠ, Zoltán**. Preparation and photocatalytic activity of TiO2 nanotube arrays prepared on transparent spinel substrate. In Ceramics International, 2021, vol. 47, no. 9, p. 12970-12980. (2020: 4.527 - IF, Q1 - JCR, 0.936 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.ceramint.2021.01.160
9. **KIM, Young-Wook - KULTAYEVA, Shynar - SEDLÁČEK, Jaroslav - HANZEL, Ondrej - TATARKO, Peter - LENČÉŠ, Zoltán - ŠAJGALÍK, Pavol**. Thermal and electrical properties of additive-free rapidly hot-pressed SiC ceramics. In Journal of the European Ceramic Society, 2020, vol. 40, no. 2, p. 234-240. (2019: 4.495 - IF, Q1 - JCR, 1.164 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jeurceramsoc.2019.10.015**

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11. PÁLKOVÁ, Helena - ZIMOWSKA, Malgorzata - JANKOVIČ, Ľuboš - SULIKOWSKI, B. - SERWICKA, Ewa M. - MADEJOVÁ, Jana. Thermal stability of tetrabutyl-phosphonium and -ammonium exchanged montmorillonite: Influence of acid treatment. In Applied Clay Science, 2017, vol. 138, p. 63-73. (3.101 - IF2016). https://doi.org/10.1016/j.clay.2016.12.043
12. **BUJDÁK, Juraj. The effects of layered nanoparticles and their properties on the molecular aggregation of organic dyes. In Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2018, vol. 35, p. 108-133. (15.325 - IF2017).** https://doi.org/10.1016/j.jphotochemrev.2018.03.001
13. KUREKOVÁ, Valéria - BELUŠÁKOVÁ, Silvia - BOHÁČ, Peter - BUJDÁK, Juraj**. Resonance energy transfer in the systems of smectite modified with a fluorescent cationic polymer and a photosensitizer. In Applied Clay Science, 2019, vol. 183, no., p. 105326-1-105326-9. (2018: 3.890 - IF, Q1 - JCR, 0.990 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.clay.2019.105326
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15. MADEJOVÁ, Jana** - JANKOVIČ, Ľuboš - SLANÝ, Michal - HRONSKÝ, Viktor. Conformation heterogeneity of alkylammonium surfactants self-assembled on montmorillonite: Effect of head-group structure and temperature. In Applied Surface Science, 2020, vol. 503, p. 144125-1-144125-11. (2019: 6.182 - IF, Q1 - JCR, 1.230 - SJR, Q1 - SJR). https://doi.org/10.1016/j.apsusc.2019.144125

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17. PÁLKOVÁ, Helena** - BARLOG, Martin - MADEJOVÁ, Jana - HRONSKÝ, V. - PETRA, L. - ŠIMON, Erik - BILLIK, Peter - ZIMOWSKA, M. Structural changes in smectites subjected to mechanochemical activation: The effect of the occupancy of the octahedral sites. In Applied Clay Science, 2021, vol. 213, p. 106214. (2020: 5.467 - IF, Q1 - JCR, 1.062 - SJR, Q1 - SJR). https://doi.org/10.1016/j.clay.2021.106214
18. ŠIMONOVÁ, Tímea** - MÉSZÁROS, R. - SEBECHLEBSKÁ, Táňa - BUJDÁK, Juraj**. Non-Arrhenius kinetics and slowed-diffusion mechanism of molecular aggregation of a rhodamine dye on colloidal particles. In Physical Chemistry Chemical Physics, 2021, vol. 23, no. 32, p. 17177-17185. (2020: 3.676 - IF, Q1 - JCR, 1.053 - SJR, Q1 - SJR). https://doi.org/10.1039/d1cp02762j

Department of Molten Salts

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25. KORENKO, Michal** – ŠIMKO, František – MLYNÁRIKOVÁ, Jarmila – LARSON, Carol – MIKŠÍKOVÁ, Eva – PRIŠČÁK, Jozef – AMBROVÁ, Marta – PALUMBO, Robert. Physico-chemical properties of $(MgF_2\text{-}CaF_2\text{-}(LiF))_{eut}$-MgO system as a molten electrolyte for Mg electrowinning. In Journal of Molecular Liquids, 2019, vol. 275, p. 535-543. (2018: 4.561 – IF). https://doi.org/10.1016/j.molliq.2018.11.066
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calculations of the room and high temperature structures of rubidium cryolite, Rb_3AlF_6. In Inorganic Chemistry, 2020, vol. 59, no. 9, p. 6308-6318. (2019: 4.825 – IF). ISSN 0020-1669. https://doi.org/10.1021/acs.inorgchem.0c00415

Department of Theoretical Chemistry

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33. VÍCHA, Jan** – KOMOROVSKÝ, Stanislav – REPISKÝ, Michal – MAREK, Radek – STRAKA, Michal**. Relativistic spin-orbit heavy atom on the light atom NMR chemical shifts: General trends across the periodic table explained. In Journal of Chemical Theory and Computation, 2018, vol. 14, no. 6, p. 3025-3039. (2017: 5.399 – IF, Q1 – JCR, 2.497 – SJR, Q1 – SJR). ISSN 1549-9618. DOI: https://doi.org/10.1021/acs.jctc.8b00144
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Vitrum Laugaricio Department

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GATES, W.P. - PETIT, Sabine - MADEJOVÁ, Jana. Applications of NIR/MIR to determine site occupacy in smectites: Chapter 7. In Infrared and Raman spectroscopies of clay minerals. - Netherlands: Elsevier, 2017, p. 200-221. ISBN 978-0-08-100355-8. ISSN 1572-4352.

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PROTSENKO, V.** - KITYK, A. - DANILOV, F.I. - PAVLÍK, Viliam - BOČA, Miroslav. Electropolishing of metals and alloys using electrochemical systems based on environmentally safe deep eutectic solvents. In Environmentally friendly technologies : Advances in research and future directions. - New York, USA : Nova Science Publishers, Inc., 2020, p. 101-131. ISBN 978-1-53678-400-6.

SCHOLTZOVÁ, Eva**. Computational modeling of nanoclays. In Micro & Nano Technologies Series: Clay Nanoparticles.Properties and Applications. Netherlands: Elsevier, 2020, p. 139-166. ISBN 978-0-12-816783-0.

2.1.4. List of monographs/books published in Slovakia

2.1.5. List of other scientific outputs specifically important for the institute, max. 10 items for institute with less than 50 average FTE researchers per year, 20 for institutes with 50 – 100 average FTE researchers per year and so on

1. The in-house DFT program package ReSpect, which is used as a platform for implementation of newly-developed quantum chemical methods. The last public release was in 2019, version 5.1.0 [http://respectprogram.org/].
2. Two modules of the periodic DFT code VASP: (i) calculation of London dispersion interactions within semi-local DFT [https://www.vasp.at/wiki/index.php/IVDW], publicly available since version 5.2.11; (ii) advanced molecular dynamics methods [https://www.vasp.at/wiki/index.php/Category:Molecular_dynamics], publicly available since version 5.2.11.
3. A computerized measuring device (Multicomponent model for thermal analysis data collections from National Instruments, where the data collections were run online with Labview software) was developed at the Department of Molten Systems, IIC. The temperature of the sample and reference compound is controlled by Pt-PtRh10 thermocouples, calibrated on the melting points of the pure salts. The system can maintain a controlled temperature gradient over a wide temperature window (around 600^{o}C), at low cooling rates (1.0 to 2.0 °C/min).
4. Chemometric analysis has been used for the analysis of multi-component systems where basic information on the composition is missing. After basic data processing, the decomposition of spectral matrices into the spectra of the principal components and their concentrations is performed. Principal Component Analysis has been used to estimate the number of components, and Multivariate Curve Resolution (Alternating Least Square) helps to reveal the components' spectral profiles and arbitrary concentrations. In some cases, Multiple Linear

Regression can help to estimate real concentrations. We have used the methods so far to analyze complex data from UV-Vis, fluorescence and infrared spectra.

5. Porous silicon nitride-based bioceramics have been designed for trabecular bone substitutes; nonoxide bioceramic microgranules have been prepared for drug delivery.
6. A unique technology for surface modification of ceramics using an oxyacetylene flame, which can be used either for the investigation of ablation resistance of materials up to 3000°C or the creation of a porous, bioactive surface on ceramic materials.
7. Joining technology using an electric field assisted process, which significantly improves the application potential of various classes of materials by making it possible to join them to similar or dissimilar materials to form a more complex structure.
8. The identification of waste as a potential source of secondary raw material. A database of data on the existence of secondary raw materials (from the production of ferroalloys and ferrous and non-ferrous metals, magnesite, power plant ash, and municipal waste incineration plants) in Slovakia was created. The obtained database on wastes significantly improves the possibilities of their controlled use as secondary raw materials; the treatment technology can be selected more quickly, and process parameters can be set on the basis of this knowledge.
9. The upgrading of the glassy slag produced by the processing of thermal waste, in particular the production of an insulation material based on a porous glass-ceramic matrix. Types of industrially well-established mineral activators, accurate proportions when mixing the glassy slag powder from the molten slag, the fluxing agent and activators, and the operational conditions of foaming (temperature, atmosphere, compacting of the material) were optimized.
10. Translucent Y_2O_3 ceramics were prepared from commercial dry-moulded nano-powder. Nano-Y_2O_3 nanopowder with a particle size of approximately 30 nm was shaped by uniaxial pressing, compacted by pre-sintering at 1500°C and then isostatically hot pressed to produce translucent Y_2O_3 ceramics from unfired samples with a low initial density. Due to the excellent sinterability of the Y_2O_3 nanopowder, a translucent Y_2O_3 ceramic with high density was obtained.

2.1.6. List of patents, patent applications, and other intellectual property rights registered abroad

2.1.7. List of patents, patent applications, and other intellectual property rights registered in Slovakia

2.1.8. Narrative on the most important research outputs of the institute – especially focused on their importance for society (3-5 pages)

Research outputs: The typical way to quantitatively evaluate any institute is to summarise the scientometric parameters. There are a number of important factors that influence the general “productivity” in terms of publication, and the number of annual publications specifically. Within the evaluated period we can identify a number of factors, with the following being the most important:

- relatively intensive renovations of laboratories and the water and sewage systems – which means that laboratories were closed for several months,
- Covid-19 – unpredictable restrictions were applied that resulted in the interruption of experimental work several times in the last two years (surprisingly, it seems that working from home resulted in an increased number of publications),
- some natural but slightly increased fluctuation in personnel was observed, including retirement, the coming and going of young researchers (including for maternity holidays) and, fortunately, increasing numbers of PhD students,
- some other external factors, such as success in national and international projects and success in contracts with industrial partners (paradoxically, working for industrial partners may result in a decrease of publications, as often these activities are subject to confidentiality agreements).

Consequently, the number of publications fluctuates from year to year. However, in order to look at trends over time it is reasonable to divide the number of publications by the number of researchers (here, we will use the number of FTE – full-time employed – researchers). As can be seen from Table 2.1.9. the publication activity of the Institute has systematically increased each year in recent

times (except for year 2019) as regards the most significant categories in the Advanced Rapid Library (ARL) system ADC and ADD, i.e. publications in journals included in the Current Content Connect list. More importantly, however, the average publication number per FTE researcher has increased up to 1.381 in the assessment period, in comparison to the previous assessment period, where the value was 0.837 (representing a 65 % increase). The increasing trend of average publication number per FTE researcher is visible also for the other categories, AAA-ABD. On other hand, a decrease in the average publication number / FTE researcher can be seen in all "conference" categories in the current assessment period, in comparison with the previous one. This seems to be the result of the pandemic situation, as can be seen in the last two years.

The average impact factor (IF) of journals in which the Institute has published is trending upwards (see table below; data are based on annual reports), and increased from 2.71 in 2016 up to 4.32 in 2021; this is more than a 60 % increase, and a faster increase than the "natural" increase of the IF of journals. Probably a better overview is given by the median IF of journals in which the Institute published. This also shows an increasing trend, thus eliminating some extremes (which can bias the mean-average IF). The JCR Average Journal IF Percentile has the Institute reaching an average value of 77th percentile in 2021 (in the case of the median, the value is even higher, at the 79th percentile). From this point of view, we can say that the quality of the outputs in 2021 was significantly above average (we could probably show very similar results for other years as well).

IF		Number of publications (ADC and ADD)				
	2016	2017	2018	2019	2020	2021
< 1	5	5	3	1	5	1
1-2	12	11	5	8	4	2
2-3	22	8	20	6	23	17
3-4	3	19	19	12	13	21
4<	7	8	14	17	31	39
∑	**49**	**51**	**61**	**44**	**76**	**80**

*the numbers of publications might slightly differ from Table 2.1.9 as they come from annual reports

Year	2016	2017	2018	2019	2020	2021
Average IF	2.71	2.83	3.41	3.66	4.17	4.32
Median IF	2.74	3.10	3.06	3.45	3.26	3.65

The total number of citations registered in WoS and SCOPUS remains between 1300 and 1600 citations per year. The quality of the outputs is also documented by the H-index of the Institute, which for the publications published in 2016-2021 stands at 25! We consider this an outstanding result compared to other comparable institutions.

Research topics in context: The R&D activities pursued by the Institute mostly cover fundamental research, although applied and industry-oriented research also play an important role. The research topics of the Institute are mostly oriented towards inorganic materials and systems. The aim of the research is to provide a fundamental description of these materials; but there is also a considerable effort to prepare selected materials which have potential for practical usage. The objectives of the majority of the publications originating from the assessment period fall under the main research topics of the Institute, i.e. the relations between the composition, properties and structure of inorganic substances; thermodynamics and chemical reactions in inorganic systems; and the development and application of theoretical and experimental methods for the determination of the structure and properties of substances. The high levels of experience and competences of the Institute's employees keep our research topics at a level of considerable interest for the wider scientific community. It should, however, be noted that while in more scientifically-developed countries research activities are systematically supported not only by their governments but also by industry,

in Slovakia support from the latter is minimal. The lack of significant external support, and the rather limited extent of governmental support, thus seriously hampers scientific development regardless of the field of interest. As the Institute was established mainly for basic research, internationally recognised and accepted research achievements are the required “products” of the Institute activities. Due to the questionnaire limitations it is not possible to present all particularly important results. Therefore, only selected results of each department have been listed in a concise form, providing information on the importance of the results in the context of international research activity, on the role of the Institute in obtaining these results, and on the response of the scientific community. The Institute has broad international contacts with scientists all over the world, leading to international collaboration in all main research activities (see 1.8 and 2.3.1). The Institute’s generally well-regarded position in the European Research Area (ERA) is also shown by our many international or bilateral projects.

The societal impact of the activities of IIC SAS involves energy savings (development of efficient phosphors for light emitting diodes, application of molten salts for heat storage and transfer, and cooling of nuclear plants), benefits to the environment (application of modified clay minerals for waste handling, and purification of water, NMR and EPR analysis of heavy elements) and a better quality of life for the older generation (ceramic implants as bone substitutes). The participation of IIC SAS in European projects gives a chance for for small-to-medium enterprise (SMEs) from Slovakia to join these research consortia as industrial partners, be a beneficiary of achieved know-how, and make contacts with foreign companies. The participation of Slovak SMEs together with IIC in EU projects might generate new employment for young experts. The local social impact is on young researchers who have finished their PhD at IIC SAS. The high scientific level of supervisors from IIC, and the good infrastructure, enable the young researchers to gather a very broad understanding of matters from a range of disciplines (chemistry, engineering, processing, computer simulations) with an emphasis on interdisciplinary thinking, implementation and practice. These benefits should help them to find a position in well-recognized companies or research institutes.

Department of Ceramics

Development of new **low-cost space launch systems and hypersonic vehicles requires new advanced materials** with temperature capabilities well above 2000°C. Therefore, new composite materials, based on transition metal compounds with extremely high melting temperatures, are being developed at the institute. The application potential of such materials is enhanced by the development of inexpensive, reliable and user-friendly methods to join them together to form large components with complex structures. This has a significant effect on the reliability, safety, and cost efficiency of aerospace missions, as well as of commercial flights.

New additive-free SiC ceramics are being developed at the institute, which exhibit the highest thermal conductivity (164 W/m.K) and electrical conductivity (830 S/m) at room temperature ever reported for sintered SiC ceramics processed at ≤ 1900°C. These properties significantly broaden the application potential of SiC ceramics.

Ceramic phosphors: Novel nitride and oxynitride phosphors doped with rare earth elements (Eu, Ce, Sm) with high thermal stability, high efficiency and good colour rendering have been developed for high-power LEDs. The experiments were supplemented with first-principles calculations on the electronic structure of rare earth-doped ceramic phosphors.

Batteries: Intensive research effort has been devoted to the development of novel ceramic anodes for Na-ion batteries, with the goal of replacing expensive and flammable Li-ion batteries with cheaper, safer and more affordable Na-ion batteries.

Ceramic nanotubes: TiO_2 nanotube arrays were prepared on a transparent spinel substrate for photocatalytic degradation of pollutants (Rhodamine B and Bisphenol A) in water. The whole ceramic system, i.e. nanotubes on a ceramic substrate, can be deployed in very harsh environments where other systems, with less stable support, fail.

Department of Hydrosilicates

Research in the field of layered materials performed in the Department was, in the assessed period, focused on the preparation, using surface active compounds, on composite materials with potential for applications in polymer nanocomposites as fillers with flame-retardant properties. Alkylammonium and alkylphosphonium cations were intensively studied for modification of both natural and synthetic 2D materials. Later the preparation of layered materials modified with certain unique surface-active molecules was performed. Complex and multidisciplinary research led to important research outputs explaining the conformational behaviour of these cations in the interlayer space or on the edges of the layers; the dependence of thermal stability on surfactant type and size; the effects of the type of layered host and its structure on the resulting properties which may have a significant effect on practical applications. An important part of the research was the use of modified clay minerals to influence the spectral behaviour of dye molecules. The layered host acted as a carrier in the multicomponent systems, stabilising the loaded molecules, and under optimised conditions caused alteration of the luminescent properties of the dye molecules in the system. Careful design of the synthesis conditions was found to be the crucial step for reducing negative factors that may influence performance of these materials. Hybrid materials based on inorganic layered nanoparticles in the role of carriers of bioactive organic molecules, in particular photosensitizers, were also used to modify the surfaces of selected types of polymers often used in medical practise. The results showed a significant photosensitizing effect of the prepared membranes. Citation responses to the work performed in the department reflect the societal relevance of the department's research path and its strong position in the field of fundamental research of clay minerals.

Department of Molten Systems

Molten salt electrolytic systems are a potentially game-changing technology that could enable cost-competitive, safe, and more sustainable commercial electrowinning, recovery, and recycling of different kinds of metals, ranging from mass-produced aluminium, through solar-grade silicon and magnesium, to the electrowinning of rare earth elements and other critical materials (e.g. tantalum, niobium, and scandium). Besides aluminium, the above-mentioned elements are directly listed by European Commission as critical materials for EU industry. The ultimate aim of the Department of Molten Systems is to understand how the molecular-scale interactions, structure, and dynamics of molten electrolytes lead to the final macroscale physico-chemical properties (like phase equilibria, density, electrical conductivity, etc.). This research thus involves two specific aims: i) the investigation of the structure and dynamics of the molten systems, and ii) studying their electrochemical and physico-chemical behaviour. In addition to the metallurgical applications, molten salt media also play a crucial role in the production, transport, and storage of energy (heat exchange interfaces in solar and nuclear applications; molten fluoride fuels, molten fluoride blankets, and molten salt moderators in different types of molten salt reactors; molten storage media; etc.). In all the aforementioned topics, the Department of Molten Systems is a visible player in the international community, in academia as well as in industry, in Europe, USA, and China. The extent of the international cooperation of the department is evident from the number of mutual publications with our foreign partners and the scale of the projects for the industrial partners. The team of the Department proved to be highly competitive with teams from such countries as the USA, China, Japan, France, Norway, Germany, New Zealand, India, Australia, Russia and Canada.

Department of Theoretical Chemistry

For many years, one of the main lines of research of the Department has been the development of state-of-the-art relativistic methods for calculations and interpretation of the spectroscopic properties of heavy-element compounds. The developed methods have been implemented into our in-house ReSpect program, which in its current form is mainly the product of a fruitful collaboration between our Institute and the Arctic University of Norway. The new features implemented into ReSpect during the reported period include methods for the calculation of nonlinear optical properties, EPR parameters with the polarizable continuum model, chiroptical properties, electron absorption spectra and circular dichroism of both closed- and open-shell systems, X-ray spectra, radiative lifetimes, and indirect spin-spin coupling parameters of paramagnetic systems, as well as visualization of the NMR parameters. The program is freely available to the academic community (http://respectprogram.org/)

and is already used by many scientific groups in the world. The popularity of the program can be seen from the fact that an article serving as an introduction to the ReSpect program, published only two years ago, already has 25 citations.

The ReSpect program is also a powerful instrument for expanding the borders of fundamental knowledge. The interpretation tools implemented in the ReSpect program helped us to identify the rules governing relativistic heavy-neighboring-atom effects on NMR shifts. The resulting new fundamental law was developed in a series of publications, where the last article was published in a journal, *Chemical Reviews*, that has an impact factor higher than 50. The review provides guidelines to help NMR spectroscopists and computational chemists to estimate the ranges of NMR shifts for unknown compounds, identify intermediates in catalytic and other processes, analyze conformational aspects and intermolecular interactions, and predict trends in series of compounds throughout the Periodic Table. It can also can be used for education in heavy-element chemistry.

The properties of advanced materials based on clay minerals have been studied in the department for a long time by applying the *ab initio* DFT method for solid state calculations. The study of the binding of organic surfactants, which improve the hydrophobic properties of clays and the structural stability of these hybrid materials, is essential for their effective use. The new information gained from calculation is valuable as it cannot be obtained by experimental methods. For example, a detailed analysis of the computed vibrational modes enabled the distinction of the different vibrations of various functional groups in the overlapping bands of the experimental infrared spectrum. The calculated mechanical properties helped to find the most suitable organoclay for the best dispersion in the polymer matrix. Modified clays are also usable in green technologies for the remediation of contaminated water or soil as effective adsorbents of pollutants from the environment, e.g. pesticides or drugs. The published findings resulted in an invitation to write a chapter dedicated to applying computational methods to these structures.

Joint Glass Centre (Vitrum Laugaricio, acr. VILA)

The Joint Glass Centre (VILA) is one of the leaders in the Slovak Republic in the field of inorganic non-metallic materials, with special attention paid to transparent glass and ceramics as well as the development of new inorganic phosphors for LED. In the department, phosphors in the Y_2O_3-Al_2O_3 system doped with Eu^{2+}/Eu^{3+} ions have been developed. Due to the presence of both oxidation states of Eu in the matrix (Eu^{2+} emits intensely in the 400-700 nm region, i.e. across the visible spectrum, while Eu^{3+} is a typical red light emitter), white light emission can be achieved, and by tuning the wavelength of the excitation radiation, the fraction of red light emission in the resulting white light can be effectively increased. In particular, the use of only one rare earth (RE) ion, at a relatively low concentration in the matrix, is an undeniable advantage, in contrast to known phosphors where the presence of 2-3 different RE ions in one or more phases is necessary for white light emission.
Polycrystalline magnesium aluminate spinel, a cost-effective alternative to sapphire single crystals for optical applications, was successfully prepared without the typical discolouration caused by the presence of carbon. Moreover, translucent glass with the composition of yttrium aluminium garnet was first time prepared by viscous flow sintering, despite its high tendency to crystallise.
Another topic with societal impact is the chemical durability of gamma-irradiated glass fibrous insulation, commonly used in the reactor containment of nuclear power plants. The results show the extraordinary brittleness of glass fibers irradiated at high temperatures. This important new finding needs further experimental and theoretical investigation.

2.1.9. Table of research outputs

Papers from international collaborations in large-scale scientific projects (Dwarf team, ALICE Collaboration, ATLAS collaboration, CD Collaboration, H1 Collaboration, HADES Collaboration, and STAR Collaboration) have to be listed separately

Scientific publications	2016			2017			2018			2019			2020			2021			total			
	number	No. / FTE researches	No. / one million total salary budget	number	No. / FTE researches	No. / one million total salary budget	number	No. / FTE researches	No. / one million total salary budget	number	No. / FTE researches	No. / one million total salary budget	number	No. / FTE researches	No. / one million total salary budget	number	No. / FTE researches	No. /1 million total salary budget	number	averaged number per year	av. No. / FTE researches	av. No. / one million total salary budget
Scientific monographs and monographic studies in journals and proceedings published abroad *(AAA, ABA)*	0	0.000	0.000	1	0.023	0.789	0	0.000	0.000	0	0.000	0.000	1	0.025	0.622	0	0.000	0.000	**2**	**0.333**	**0.008**	**0.235**
Scientific monographs and monographic studies in journals and proceedings published in Slovakia *(AAB, ABB)*	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	**0**	**0.000**	**0.000**	**0.000**
Chapters in scientific monographs published abroad *(ABC)*	0	0.000	0.000	5	0.113	3.946	**0**	0.000	0.000	0	0.000	0.000	2	0.050	1.243	2	0.046	1.214	**9**	**1.500**	**0.035**	**1.059**
Chapters in scientific monographs published in Slovakia *(ABD)*	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000		0.000	0.000	**0**	**0.000**	**0.000**	**0.000**
Scientific papers published in journals registered in Current Contents Connect *(ADCA, ADCB, ADDA, ADDB)*	49	1.068	43.058	52	1.173	41.042	57	1.239	41.304	43	1.056	29.452	78	1.941	48.477	81	1.862	49.180	**360**	**60.000**	**1.381**	**42.348**
Scientific papers published in journals registered in Web of Science Core Collection and SCOPUS not listed above *(ADMA, ADMB, ADNA, ADNB)*	7	0.153	6.151	5	0.113	3.946	4	0.087	2.899	6	0.147	4.110	5	0.124	3.108	4	0.092	2.429	**31**	**5.167**	**0.119**	**3.647**
Scientific papers published in other foreign journals (not listed above) *(ADEA, ADEB)*	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	**0**	**0.000**	**0.000**	**0.000**
Scientific papers published in other domestic journals (not listed above) *(ADFA, ADFB)*	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	**0**	**0.000**	**0.000**	**0.000**
Scientific papers published in foreign peer-reviewed proceedings *(AECA)*	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	**0**	**0.000**	**0.000**	**0.000**
Scientific papers published in domestic peer-reviewed proceedings *(AEDA)*	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	0	0.000	0.000	**0**	**0.000**	**0.000**	**0.000**
Published papers (full text) from foreign scientific conferences *(AFA, AFC)*	2	0.044	1.757	5	0.113	3.946	4	0.087	2.899	5	0.123	3.425	2	0.050	1.243	4	0.092	2.429	**22**	**3.667**	**0.084**	**2.588**
Published papers (full text) from domestic scientific conferences *(AFB, AFD)*	18	0.392	15.817	9	0.203	7.103	9	0.196	6.522	18	0.442	12.329	0	0.000	0.000	1	0	1	**55**	**9**	**0**	**6**

2.2. Measures of research outputs (citations, etc.)

2.2.1. Table with citations per annum (without self-citations)

Citations of papers from international collaborations in large-scale scientific projects (Dwarf team, ALICE Collaboration, ATLAS collaboration, CD Collaboration, H1 Collaboration, HADES Collaboration, and STAR Collaboration) are listed separately

Citations, reviews	2015		2016		2017		2018		2019		2020		total		
	number	No. / FTE researchers	number	No. / FTE researchers	number	No. / FTE researchers	number	No. / FTE researchers	number	No. / FTE researchers	number	No. / FTE researchers	number	averaged number per year	av. No. / FTE researchers
Citations in Web of Science Core Collection (1.1, 2.1)	1,350	29.42	1,420	32.03	1,693	36.80	1,647	40.46	1,694	42.16	1,870	42.98	**9,674**	**1,612.33**	**37.12**
Citations in SCOPUS (1.2, 2.2) if not listed above	127	2.77	30	0.68	22	0.48	33	0.81	29	0.72	22	0.51	**263**	**43.83**	**1.01**
Citations in other citation indexes and databases (not listed above) (3.2,4.2)	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	0	0.00	**0**	**0.00**	**0.00**
Other citations (not listed above) (3.1, 4.1)	0	0.00	0	0.00	3	0.07	2	0.05	1	0.02	1	0.02	**7**	**1.17**	**0.03**
Reviews (5,6)	0	0.00	1	0.02	0	0.00	0	0.00	0	0.00	0	0.00	**1**	**0.17**	**0.00**

2.2.2. List of 10 most-cited publications published any time with the address of the institute, with number of citations in the assessment period (2015 – 2020)

HELGAKER, Trygve - KLOPPER, Wim - KOCH, Henrik - NOGA, Jozef. Basis-set convergence of correlated calculations on water. In Journal of Chemical Physics, 1997, vol. 106, no. 23, p. 9639-9646. (1996: 3.516 - IF, CCC). **Number of citations: 625**

MADEJOVÁ, Jana. FTIR techniques in clay mineral studies. In Vibrational Spectroscopy, 2003, vol. 31, no. 1, p. 1-10. https://doi.org/10.1016/S0924-2031(02)00065-6

Number of citations: 600

MADEJOVÁ, Jana - KOMADEL, Peter. Baseline studies of The Clay Minerals Society Source Clays: Infrared methods. In Clays and Clay Minerals, 2001, vol. 49, no. 5, p. 410-432. (2001 - Current Contents). ISSN 0009-8604. https://doi.org/10.1346/CCMN.2001.0490508

Number of citations: 403

SCHLEYER, P.V. - JIAO, H.J. - HOMMES, N.J.R.V. - MALKIN, Vladimír - MALKIN, Oľga. An evaluation of the aromaticity of inorganic rings: Refined evidence from magnetic properties. In Journal of the American Chemical Society, 1997, vol. 119, no. 51, p. 12669-12670.

Number of citations: 182

BUČKO, Tomáš - LEBÈGUE, Sébastien - HAFNER, Jürgen - ÁNGYÁN, János G. Tkatchenko-Scheffler van der Waals correction method with and without self-consistent screening applied to solids. In Physical Review B, 2013, vol. 87, no. 6, p. 064110-1-064110-15. (2012: 3.767 - IF, Q1 - JCR, 1.779 - SJR, Q1 - SJR, CCC). (https://doi.org/10.1103/PhysRevB.87.064110

Number of citations: 167

KAUPP, Martin - MALKIN, Oľga - MALKIN, Vladimír - PYYKKÖ, Pekka. How do spin-orbit-induced heavy-atom effects on NMR chemical shifts function? Validation of a simple analogy to spin-spin coupling by density functional theory (DFT) calculations on some iodo compounds. In Chemistry - A European Journal, 1998, vol. 4, no. 1, p. 118-126. ISSN 0947-6539.

Number of citations: 115

NOGA, Jozef - BARTLETT, Rodney J. The full CCSDT model for molecular electronic structure. In Journal of Chemical Physics, 1987, vol. 86, no. 12, p. 7041-7050. ISSN 0021-9606.

Number of citations: 105

BARTLETT, Rodney J. - WATTS, J. D. - KUCHARSKI, Stanislaw A. - NOGA, Jozef. Non-iterative fifth-order triple and quadruple excitation energy corrections in correlated methods. In Chemical Physics Letters, 1990, vol. 165, no. 6, p. 513-522. https://doi.org/10.1016/0009-2614(90)87031-L

Number of citations: 101

BUČKO, Tomáš - LEBÈGUE, Sébastien - ÁNGYÁN, János G. - HAFNER, Jürgen. Extending the applicability of the Tkatchenko-Scheffler dispersion correction via iterative Hirshfeld partitioning. In Journal of Chemical Physics, 2014, vol. 141, p. 034114-1-034114-17. (2013: 3.122 - IF, Q1 - JCR, 1.532 - SJR, Q1 - SJR, CCC). https://doi.org/10.1063/1.4890003

Number of citations: 89

KOMADEL, Peter. Acid activated clays: Materials in continuous demand. In Applied Clay Science, 2016, vol. 131, p. 84-99. (2015: 2.586 - IF, Q1 - JCR, 0.806 - SJR, Q2 - SJR, CCC). (2016 - Current Contents). https://doi.org/10.1016/j.clay.2016.05.001

Number of citations: 84

2.2.3. List of 10 most-cited publications published any time with the address of the institute, with number of citations obtained until 2020

HELGAKER, Trygve - KLOPPER, Wim - KOCH, Henrik - NOGA, Jozef. Basis-set convergence of correlated calculations on water. In Journal of Chemical Physics, 1997, vol. 106, no. 23, p. 9639-9646. (1996: 3.516 - IF, CCC). (1997 - Current Contents, WOS, SCOPUS, WOS, SCOPUS)..

Number of citations: 1381

MADEJOVÁ, Jana. FTIR techniques in clay mineral studies. In Vibrational Spectroscopy, 2003, vol. 31, no. 1, p. 1-10. https://doi.org/10.1016/S0924-2031(02)00065-6

Number of citations: 1016

MADEJOVÁ, Jana - KOMADEL, Peter. Baseline studies of The Clay Minerals Society Source Clays: Infrared methods. In Clays and Clay Minerals, 2001, vol. 49, no. 5, p. 410-432. (2001 - Current Contents). https://doi.org/10.1346/CCMN.2001.0490508

Number of citations: 645

SCHLEYER, P.V. - JIAO, H.J. - HOMMES, N.J.R.V. - MALKIN, Vladimír - MALKIN, Oľga. An evaluation of the aromaticity of inorganic rings: Refined evidence from magnetic properties. In Journal of the American Chemical Society, 1997, vol. 119, no. 51, p. 12669-12670. ISSN 0002-7863.

Number of citations: 483

NOGA, Jozef - BARTLETT, Rodney J. The full CCSDT model for molecular electronic structure. In Journal of Chemical Physics, 1987, vol. 86, no. 12, p. 7041-7050. ISSN 0021-9606.

Number of citations: 337

BARTLETT, Rodney J. - WATTS, J. D. - KUCHARSKI, Stanislaw A. - NOGA, Jozef. Non-iterative fifth-order triple and quadruple excitation energy corrections in correlated methods. In Chemical Physics Letters, 1990, vol. 165, no. 6, p. 513-522. https://doi.org/10.1016/0009-2614(90)87031-L

Number of citations: 289

URBAN, Miroslav - NOGA, Jozef - COLE, S.J. - BARTLETT, Rodney J. Towards a full CCSDT model for electron correlation. In Journal of Chemical Physics, 1985, vol. 83, no. 8, p. 4041-4046. ISSN 0021-9606.

Number of citations: 230

BUČKO, Tomáš - LEBÈGUE, Sébastien - HAFNER, Jürgen - ÁNGYÁN, János G. Tkatchenko-Scheffler van der Waals correction method with and without self-consistent screening applied to solids. In Physical Review B, 2013, vol. 87, no. 6, p. 064110-1-064110-15. (2012: 3.767 - IF, Q1 - JCR, 1.779 - SJR, Q1 - SJR, CCC). https://doi.org/10.1103/PhysRevB.87.064110

Number of citations: 202

KAUPP, Martin - MALKIN, Oľga - MALKIN, Vladimír - PYYKKÖ, Pekka. How do spin-orbit-induced heavy-atom effects on NMR chemical shifts function? Validation of a simple analogy to spin-spin coupling by density functional theory (DFT) calculations on some iodo compounds. In Chemistry - A European Journal, 1998, vol. 4, no. 1, p. 118-126. ISSN 0947-6539.

Number of citations: 197

MADEJOVÁ, Jana - BUJDÁK, Juraj - JANEK, Marián - KOMADEL, Peter. Comparative FT-IR study of structural modifications during acid treatment of dioctahedral smectites and hectorite. In Spectrochimica Acta Part A - Molecular and Biomolecular Spectroscopy, 1988, vol. 54, no. 10, p. 1397-1406. ISSN 1386-1425. **Number of citations: 177**

2.2.4. List of 10 most-cited publications published during the evaluation period (2016-2021) with the address of the Institute, with number of citations obtained until 2021

KOMADEL, Peter. Acid activated clays: Materials in continuous demand. In Applied Clay Science, 2016, vol. 131, p. 84-99. (2015: 2.586 - IF, Q1 - JCR, 0.806 - SJR, Q2 - SJR, CCC). (2016 - Current Contents). ISSN 0169-1317. https://doi.org/10.1016/j.clay.2016.05.001

Number of citations: 117

SLANÝ, Michal** - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana. Structural characterization of organo-montmorillonites prepared from a series of primary alkylamines salts: Mid-IR and near-IR study. In Applied Clay Science, 2019, vol. 176, p. 11-20. (2018: 3.890 - IF, Q1 - JCR, 0.990 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.clay.2019.04.016

Number of citations: 92

BUČKO, Tomáš - LEBÈGUE, Sébastien - GOULD, Tim - ÁNGYÁN, János G. Many-body dispersion corrections for periodic systems: an efficient reciprocal space implementation. In Journal of Physics: Condensed Matter, 2016, vol. 28, no. 4, p. 045201-1-045201-13. (2015: 2.209 - IF, Q2 - JCR, 1.043 - SJR, Q1 - SJR, CCC). https://doi.org/10.1088/0953-8984/28/4/045201

Number of citations: 67

MADEJOVÁ, Jana - GATES, W.P. - PETIT, Sabine. IR spectra of clay minerals : Chapter 5. In Infrared and Raman spectroscopies of clay minerals. Netherlands: Elsevier, 2017, p. 107-149. ISBN 978-0-08-100355-8. https://doi.org/10.1016/B978-0-08-100355-8.00005-9

Number of citations: 65

PATEL, Niketan Sarabhai - PAVLÍK, Viliam - BOČA, Miroslav. High-temperature corrosion behavior of superalloys in molten salts - A review. In Critical Reviews in Solid State and Materials Sciences, 2017, vol. 42, no. 1, p. 83-97. (2016: 6.455 - IF, Q1 - JCR, 1.924 - SJR, Q1 - SJR, CCC). https://doi.org/10.1080/10408436.2016.1243090

Number of citations: 53

YADAV, S.** - KUŘITKA, Ivo - HAVLICA, Jaromír - HNATKO, Miroslav - CIGÁŇ, Alexander - MASILKO, J. - KALINA, L. - HAJDÚCHOVÁ, M. - RUSNÁK, Jaroslav - ENEV, V. Structural, magnetic, elastic, dielectric and electrical properties of hot-press sintered Co1-xZnxFe2O4 (x=0.0, 0.5) spinel ferrite nanoparticles. In Journal of Magnetism and Magnetic Materials, 2018, vol. 447, p. 48-57. (2017: 3.046 - IF, Q2 - JCR, 0.786 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jmmm.2017.09.033

Number of citations: 50

TAIFAN, William E. - BUČKO, Tomáš - BALTRUSAITIS, Jonas. Catalytic conversion of ethanol to 1,3-butadiene on MgO: A comprehensive mechanism elucidation using DFT calculations. In Journal of Catalysis, 2017, vol. 346, p. 78-91. (2016: 6.844 - IF, Q1 - JCR, 2.451 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jcat.2016.11.042

Number of citations: 42

WANG, Quan - SHAHEEN, Sabry M. - JIANG, Yahui - LI, Ronghua - SLANÝ, Michal - ABDELRAHMAN, Hamada - KWON, Eilhann - BOLAN, Nanthi - RINKLEBE, Jörg - ZHANG, Zengqiang**. Fe/Mn- and P-modified drinking water treatment residuals reduced Cu and Pb phytoavailability and uptake in a mining soil. In Journal of Hazardous Materials, 2021, vol. 403, p.123628-1-123628-9. (2020: 10.588 - IF, Q1 - JCR, 2.034 - SJR, Q1 - SJR, CCC). https://doi.org/10.1016/j.jhazmat.2020.123628

Number of citations: 42

GOULD, Tim - LEBÈGUE, Sébastien - ÁNGYÁN, János G. - BUČKO, Tomáš. A fractionally ionic approach to polarizability and van der Waals many-body dispersion calculations. In Journal of Chemical Theory and Computation, 2016, vol. 12, no. 12, p. 5920-5930. (2015: 5.301 - IF, Q1 - JCR, 2.702 - SJR, Q1 - SJR, CCC). https://doi.org/10.1021/acs.jctc.6b00925

Number of citations: 39

DU, Weichao** - SLANÝ, Michal* - WANG, Xiangyun - CHEN, Gang - ZHANG, Jie. The inhibition property and mechanism of a novel low molecular weight zwitterionic copolymer for improving wellbore stability. In Polymers : Open Access Polymer Science Journal, 2020, vol. 12, no. 3, p. 708-1-708-13. (2019: 3.426 - IF, Q1 - JCR, 0.704 - SJR, Q1 - SJR, CCC). https://doi.org/10.3390/polym12030708 **Number of citations: 39**

2.2.5. List of most-cited authors from the Institute (at most 10 % of average FTE researchers per year) and their number of citations in the assessment period (2015– 2020). The cited papers must bear the address of the institute

1. Jana Madejová 2282 (from 107 documents)
2. Peter Komadel 1706 (from 90 documents)
3. Jozef Noga 1413 (from 71 documents)
4. Pavol Šajgalík 1120 (from 142 documents)
5. Oľga Malkin 1072 (73 documents)

Note: The other two researcher reached more than 900 citations for their publications.

2.2.6. List of most-cited authors from the Institute (at most 10 % of average FTE researchers per year) and their number of citations obtained until 2020. The cited papers must bear the address of the Institute

1. Jana Madejová 4128 (115 documents)
2. Jozef Noga 3798 (92 documents)
3. Peter Komadel 3415 (101 documents)
4. Oľga Malkin 2722 (85 documents)
5. Vladimír Malkin 2460 (69 documents)
6. Pavol Šajgalík 2092 (183 documents)

Note: The other three researcher reached more than 900 citations for their publications

2.2.7. List of most-cited authors from the Institute (at most 10 % of average FTE researchers per year) and their number of citations obtained until 2021 of their papers published during the evaluation period (2016– 2021). The cited papers must bear the address of the Institute

1. Michal Slaný 284 (10 documents)
2. Tomáš Bučko 277 (17 documents)
3. Jana Madejová 271 (14 documents)
4. Dušan Galusek 212 (36 documents)
5. Ľuboš Jankovič 184 (12 documents)
6. Pavol Šajgalík 180 (24 documents)

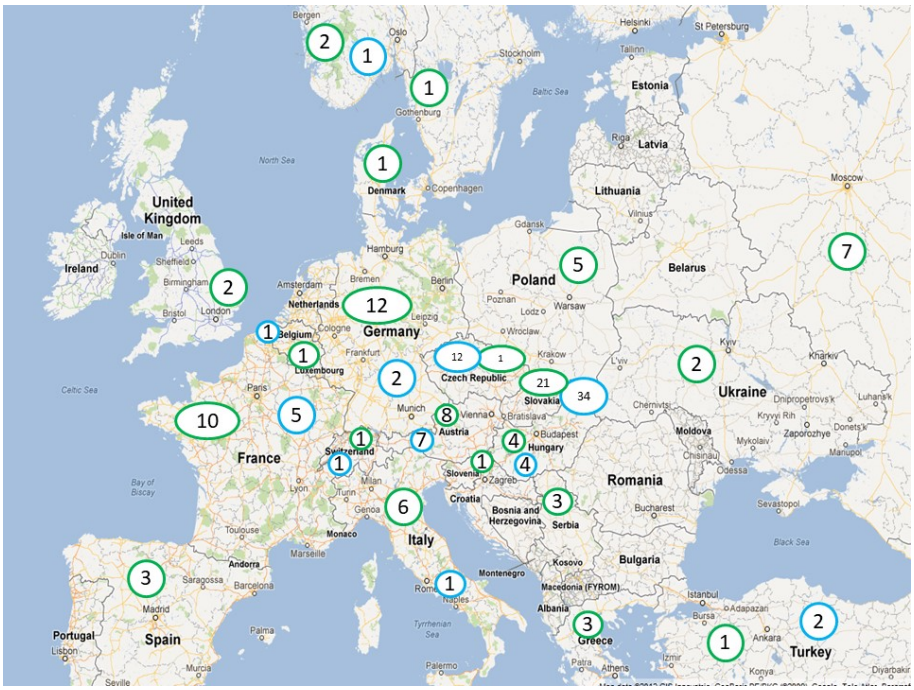
Note: The other four researcher reached more than 100 citations for their publications

2.3. Research status of the institute in international and national context

- **International/European position of the institute**

2.3.1. List of the most important research activities demonstrating the international relevance of the research performed by the institute, incl. major projects (details of projects should be supplied under Indicator 2.4). Max. 10 items for institute with less than 50 average FTE researchers per year, max. 20 for institutes with 50 – 100 average FTE researchers per year and so on

The figure below shows the distribution of collaborations with **academic (green circles**) and **industrial (blue circles**) partners all around the world (the complete list is in section 3). This list details only cooperation resulting in joint publications, projects or extended research activities within the period 2016-2021. From this extended cooperation, the following research activities have been selected to demonstrate the international relevance of the Institute's work:



1. **Participation in multilateral projects in the assessed period**
   - Horizon 2020 Sodium-Ion and Sodium Metal Batteries for efficient and sustainable next-generation energy storage, 963542, SIMBA (8 countries involved in project)
   - FP7 Marie Curie Action: Initial Training Network Pushing the envelope of nuclear magnetic resonance spectroscopy for paramagnetic systems. A combined experimental and theoretical approach (pNMR) (10 european countries participated)
   - Building a Centre of Excellence for Advanced Materials Application (CEMEA). Four institutions from SAS participated in this project with a partner from Finland (Teknologian tutkimuskeskus VTT OyEspo, HELSINGIN YLIOPISTO).
   - Two COST projects: Our astro-chemical history (institutions from 8 countries), New generation biomimetic and customized implants for bone engineering (18 countries worldwide were involved in the project)
   - Two ERA-net projects – the expertise of researchers at IIC SAS led to invitations to participate in tasks involved in already-running projects
2. **Most important results of international cooperation**
   - The development of new and reliable joining techniques for ceramic materials performing in extreme environments (such as high temperature, or nuclear) has been carried out in collaboration with Ningo Institute of Materials Technology and Engineering in China, and Politecnico di Torino in Italy.
   - New advanced ceramic materials for extreme applications, including fiber-reinforced ceramic matrix composites and ultra-high temperature ceramics, have been (and are still being) developed in collaboration with Queen Mary University of London in the UK and the Institute of Physics of Materials in the Czech Republic.
   - There is an active collaboration with University of Seoul, Korea (prof. Young-Wook Kim) on the development of SiC-based ceramics with exceptional electrical and thermal conductivity.
   - Unique synergy of measurement of macroscopic physico-chemical properties (IIC) and a microscopic structural approach using NMR spectroscopy (CEMHTI CNRS, Orléans, France) in research on molten fluorides at high temperatures.
   - Systematic and complex research on special ternary fluorides (e.g. Zr, Nb, Ta, Hf) including structural (Prof. Armel Le Bail, Université du Maine, Le Mans, France) analysis based on synchrotron radiation data, as well as multiphase solid-solid transformations analysis using spectral (CEMHTI CNRS, Orléans, France) and thermochemical methods (IIC).
3. **Researcher mobility**
   - Invited lectures at international conferences (> 80 lectures)
   - Short-term and long-term research stays at institutions within the framework of projects, based on invitations or via fellowships; broad international mobility from other countries and performance of part of the research at the IIC SAS. 32 visits of researchers including PhD students were made during the years 2016-2021 at the Institute as part of bilateral and multilateral projects, with an average length of 47 days.

List of researchers/PhD. students staying at the IIC more than 10 days

Austria	Christina Atzenhofer	32	2016
	Christina Atzenhofer	31	2018
	Christina Atzenhofer	27	2019
China	Shuang Wu	181	2019
Czech Republic	Lenka Blahová	97	2017
	Luca Bertolla	12	2019
Great Britain	Peter Cherry	275	2019
Greece	Eleni Gianni	93	2019
India	Shirshendu Chakraborty	91	2018
Pakistan	Syed Awais Rouf	91	2016
Poland	Malgorzata Zimowska	11	2016
	Malgorzata Zimowska	11	2017
	Malgorzata Zimowska	19	2018
	Malgorzata Zimowska	21	2021
Russia	Igor Petrushenko, PhD	30	2016

	Igor Petrushenko, PhD	30	2019
	Artem Kuznetsov Borisovich	61	2018
Turkey	Nadide Fulden Onan	89	2017
	Cemile Gizem Toksőz	80	2018
Ukraine	Anna Kityk	62	2018
	Anna Kityk	125	2019
	Anna Kityk	121	2020

2.3.2. List of international conferences (co)organised by the institute

9th Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria,
23. - 28. 02. 2016
Number of participants: 45 researchers from Germany, Norway, Denmark, Czech Republic, Austria, Switzerland, 27 lectures were presented.

8th Mid-European Clay Conference (MECC), Košice, Slovakia,
04. - 08. 07. 2016
Number of participants: 170 from 29 countries. 70 lectures were presented (4 invited, 6 keynote), 87 posters.

Preparation and properties of progressive ceramic materials, Košická Belá, Ružín, 23.11-25.11.2016, Number of participants: 46 from Slovak and Czech institutions. 23 lectures were presented.

10th Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria
05. - 10. 03. 2017
Number of lectures: 28, number of participants: 56 (from Germany, France, Czech Republic, Denmark, Finland, Japan, Slovakia.

11th Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria
25. 02. - 02. 03. 2018
Number of lectures: 25, number of participants: 47 from Norway, Czech Republic, Germany, Finland, Denmark, Slovakia.

9th Workshop Interactions of molten systems with progressive inorganic materials, Borinka, Slovakia
15. - 16. 10. 2018
Four institutions participated to this workshop (IIC SAS Bratislava, Faculty of Chemical and Food Technology Slovak University of Technology Bratislava, Technical University Košice TUKE a VŠB-TUO Ostrava, Czech Republic), 24 participants, 11 lectures.
IIC SAS – main organizing institution

XIIth Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria
11. - 15. 03. 2019
21 lectures, 45 participants (Germany, Slovakia, Czech Republic, Norway, USA, Switzerland

Engineering Ceramics 2019 – Ceramics for People, Smolenice, Slovakia
12. -16. 05. 2019
86 participants from 16 countries
The main focus of the conference was devoted to the preparation and characterisation of ceramic materials for improvement of the living standards of population, healthcare, (bioceramic implants, drug delivery, materials for smart diagnostics), environment (carbon nanostructures, MXenes, MBenes, porous ceramics, etc. for improved gas sensitivity and selectivity, particulate filters), materials for energy efficient and eco-friendly technologies (e.g. LEDs, energy conversion/storage, ceramics for fusion reactors, additive manufacturing), housing, transportation (including UHTCs), and engineering ceramics armed with their functional properties applied in various fields of

development.

Processing and properties of advanced ceramics and glasses, Ráztočno, Slovakia
20. -22. 11. 2019
Number of participants: 46 from Slovak and Czech institutions, scientific seminar of IIC SAS, Institute of Materials Research of SAS, VILA Trenčín, Faculty of Chemical and Food Technology Slovak University of Technology Bratislava, MUNI Brno, Czech Republic, CEITEC Brno, Czech Republic). 30 lectures were given at the event.

XIIIth Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria, 01.03.-06.03.2020
40 participants from Germany, Slovakia, Czech republic, Norway, Denmark, Austria

14th International Conference on Solid State Chemistry (SSC 2021)
14.-17.6. 2021
The Number of lectures: 65, number of posters: 13. The participants from Slovakia, Spain, Lebanon, Germany, Russia, Italy, Czech Republic, Poland, France, Hungary, Turkey, Japan, Latvia, UK, Romania. Selected contributions published in the special issue of the Journal Pure and Applied Chemistry.
IIC SAS: co-organizing institution

2.3.3. List of edited proceedings from international scientific conferences

1. Workshop Processing and properties of advanced ceramics; November 23-25, 2016, Ružín, Slovak Republic: Book of extended abstracts. Editor Jana Valúchová; reviewers Dušan Galusek, Karel Maca, Zoltán Lenčéš, Miroslav Hnatko, Jaroslav Sedláček, Marián Mikula, Alexandra Kovalčíková. Publisher: Institute of Inorganic Chemistry SAS, Bratislava, Slovakia, 2016. p. 108 ISBN 978-80971648-5-0
2. Workshop Processing and properties of advanced ceramics and glasses, November 20 - 22, 2019, Ráztočno, Slovak Republic: Book of extended abstracts. Editor Jana Valúchová; reviewers Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Michálková, Jozef Ráheľ, Peter Tatarko. Publisher: Institute of Inorganic Chemistry SAS, Bratislava, Slovakia, 2019. 149 p. ISBN 978-80-971648-8-1.
3. Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for People, Smolenice castle, May 12-16, 2019: Book of abstracts. Eds. Zoltán Lenčéš, Jana Valúchová. Publisher: Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia, 2019. 91 p. ISBN 978-80-971648-7-4.

2.3.4. List of journals edited/published by the institute and information on their indexing in WOS, SCOPUS, other database or no database, incl. impact factor and other metrics of journals in each year of the assessment period

Although institute did not edit/publish journals, several of the employees are engaged as members of editorial boards in journals indexed in WOS and/or Scopus database.

M. Boča
− Chemical Papers (member of Editorial Advisory board since 2/2006; associate editor for Inorganic Chemistry, since 6/2006-09/2013)

M. Drábik
− Ceramics-Silikáty (member)
− Pure and Applied Chemistry (conference editor SSC2014)

D. Galusek
− Ceramics-Silikáty (member)

− International Journal of Applied Ceramic Technology (associate editor)
− Journal of the European Ceramic Society
− New Journal of Glass and Ceramics

P. Komadel
− Applied Clay Science (member)
− Clay Minerals (member)
− Geologica Carpathica (member)

Z. Lenčéš
International Journal of Applied Ceramic Technology
Journal of the Ceramic Society of Japan (associate editor)

M. Liška
− Ceramics - Silikáty (member)
− European Journal of Glass Science and Technology (regional editor)
− International Journal of Applied Glass Science (member)
− Sklář a keramik (member)

J. Madejová
− Clays and Clay Minerals (associate editor)

P. Šajgalík
− Ceramics - Silikáty (member)
− Journal of Ceramic Science and Technology (member)
− Journal of Asian Ceramic Society (co-editor)
− Keramický Zpravodaj (member)
− Key Engineering Materials (member of International Advisory Board)
− Processing and Application of Ceramics (member)

P. Tatarko
− International Journal of Applied Ceramic Technology (associate editor)
− Materials

- **National position of the institute**

2.3.5. List of selected activities of national importance

1. The aim of the cooperation with Považská cementáreň, Ladce j.s.c. (producer of cements in Slovakia), is to optimize the key parameters of the production process of ceramic materials with the addition of a special cement (H-CEMENT). Finding the optimal amount of special cement and firing conditions have so far brought significant improvements in terms of reducing the energy intensity of the production process of ceramic materials while increasing the mechanical properties. The obtained results could provide significant improvement in energy savings and consequently in reducing the carbon footprint of the production of traditional ceramic materials.
2. Collaboration on the development of transparent / luminescent polycrystalline ceramic materials (TKMs) that can successfully replace glass (better mechanical properties) and single crystals (lower production costs) in the production of rigid lasers, scintillators, or electro-optical devices. Activities are focused on all stages of preparation of TKMs based on yttrium oxide and yttrium-aluminum garnet doped with optically-active ingredients. Collaboration with CEIT Technical Innovation, s.r.o., a member of CEIT group, Žilina.
3. Collaboration on the eco-friendly and resource-saving electrochemical surface treatment in a deep eutectic solvent based on vitamin B4, which could become a real breakthrough in the field of creating highly efficient surface treatment technologies for biomedical titanium alloys, which

are used for producing prostheses and implants. The collaboration was with Biomedical Engineering, a producer of Ti_6Al_4V alloy medical implants fabricated by 3D printing.

4. The long-standing collaboration of Institute with RONA Glassworks, j.s.c. Lednické Rovne. Together they implement research grants for the development of new compositions of crystalline glasses produced by the company, as well as current problems of applied research and experimental development satisfying the immediate needs of the company. Experts from RONA, j.s.c. serve as co-supervisors for doctoral students in the VILA centre.
5. Cooperation with VUEZ, j.s.c., Levice. Joint research projects aimed at determining the resistance of glass fibres used as thermal insulation in nuclear power plants to leaching in aqueous environments (Grant No. DSR/SESPRI/04s029a Chemical Effects and Chemical Effects II, funded by IRSN, France; a similar project is funded by Allion Science USA) were carried out.
6. Developing a methodology involving near-infrared spectroscopy for tracking water content in an industrially important rock (perlite) for a company mining this material. Perlite is an important raw material, deposits of which occur around the world, including in Slovakia. A new, innovative method based on near-IR spectroscopy was developed for determination of water content in perlites, an important parameter for their industrial application. The internal standards hexadecyltrimethylammonium bromide (HDTMA) and talc were used to quantify the amount of water by using the area of the H_2O combination band. The new method is fast, and in contrast to thermal analysis allows molecular water to be distinguished from structurally-bonded OH groups, and therefore has potential for application in industry.

2.3.6. List of journals (published only in the Slovak language) edited/published by the institute and information on their indexing in WOS, SCOPUS, other database or no database, incl. impact factor and other metrics of journals in each year of the assessment period

- **Position of individual researchers in the international context**

2.3.7. List of invited/keynote presentations at international conferences, as documented by programme or invitation letter

2016

D. GALUSEK: Aluminate glasses based luminescent nanomaterials for HB-LEDs, International Conference on Advances in Applied Mathematic, Materials Science and Nanotechnology for Engineering and Industrial Applications, Federal Institute of Science and Technology, Angamaly, India. Key Note lecture, 7. – 9. 1. 2016

R. KLEMENT, K. HALADEJOVÁ, P. VETEŠKA, S.-J. SHIH, W.-H. TUAN, and D. GALUSEK, Visible Broadband Luminescence of Transition Metals Doped Aluminates and Aluminosilicates, The 10th Asian Meeting on Electroceramics AMEC2016, Taipei, Taiwan, Key note lecture, 4. – 7. 12. 2016

O. MALKIN: New tools for interpretation of indirect nuclear spin-spin couplings, 6th Annual Meeting of the St. Andrew Centre of Magnetic Resonance, St. Andrews, UK, 6. 6. 2016

P. ŠAJGALÍK: Additive-free hot-pressed silicon carbide ceramics – a material with exceptional mechanical properties, CENERGY (synergy) – Materials Day 2016, Ceramics for Energy, Darmstadt, Germany, 29. 04. 2016

P. ŠAJGALÍK: Silicon nitride-hydroxyapatite bioactive composite. 6th International Congress on Ceramics: from Lab to Fab (ICC6), Dresden, Germany, 21. – 25. 8. 2016

P. ŠAJGALÍK: Additive-free hot-pressed silicon carbide ceramics - a material with exceptional mechanical properties. 91st DKG Annual Meeting in Conjunction with the Symposium on High-Performance Ceramics, TU Bergakademie Freiberg, Germany, 7. – 9. 3. 2016

P. ŠAJGALÍK: Additive-free hot-pressed silicon carbide ceramics - a material with exceptional properties. 4th International Symposium on New Frontier of Advanced Si-based Ceramics and

Composites (ISASC 2016), Haeundae Grand Hotel, Busan, Korea, 25. – 28. 9. 2016

P. ŠAJGALÍK: GB chemistry of silicon nitride based ceramics - implications to the ceramics properties. Conference on the Science and Engineering of Oxide Materials (CONSILOX XII), Sinaia, Romania, 16. – 20. 9. 2016

P. ŠAJGALÍK: In situ formed SiC nano-inclusions in Si_3N_4 based ceramics - thermal shock resistance, wear behavior and oxidation resistance. 40th International Conference & Exposition on Advanced Ceramics and Composites (ICACC 2016), Daytona Beach, Florida, USA, 24. – 29. 1. 2016

2017

J. BUJDÁK, Photofunctional hybrid materials based on layered silicates and organic dye molecules. Second International Conference on Material Science (ICMS2017), Tripura University, Agartala, India, 17. 2. 2017.

A. PRNOVÁ, J. CHOVANEC, A. PLŠKO, R. KLEMENT, D. GALUSEK, Crystallization of Aluminate and Aluminosilicate Glasses. 2017 ICG Annual Meeting and 32nd Sisecam Glass Symposium, Istanbul, Turkey, 22. – 25.10.2017

K. DRDLIKOVA, D. DRDLIK, R. KLEMENT, K. MACA, D. GALUSEK, Two stage sintering – does it work for alumina? International Conference on Sintering 2017, San Diego, USA, 12. – 16. 11. 2017

S. KOMOROVSKÝ, A new quantum number for the many-electron Dirac–Coulomb Hamiltonian, Xth Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria, 6. 3. 2017.

S. KOMOROVSKÝ, New quantum number for the many-electron Dirac-Coulomb Hamiltonian: Theory and first applications", 12th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics (REHE), Marburg, Germany, 4. 9. 2017

Z. LENČÉŠ, I. IBRAHIM, P. ŠAJGALÍK, Ľ. BENCO. Experimental and theoretical approach to lanthanide-doped LaSi3N5 phosphors. 41st International Conference and Exposition on Advanced Ceramics and Composites (ICACC 2017), Hilton Daytona Beach Resort and Ocean Center, Daytona Beach, Florida, USA, 22. – 27. 1. 2017

O. MALKIN, How to analyze the hyperfine deformation density? Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria, 7. – 9. 3. 2017

O. MALKIN, Visualization of EPR hyperfine coupling pathways. International Symposium - Theoretical Design of Materials with Innovative Functions Based on Element Strategy and Relativistic Electronic Theory, Tokyo, Japan, 8 – 9. 12. 207

V. MALKIN, Visualization of EPR hyperfine coupling pathways. Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria, 7. – 9. 3. 2017

V. MALKIN, Calculations of the EPR parameters using unrestricted two- and four-component relativistic approaches within the HF and DFT frameworks, International Symposium - Theoretical Design of Materials with Innovative Functions Based on Element Strategy and Relativistic Electronic Theory, Tokyo, Japan, 8 – 9. 12. 2017

J. NOGA, Pair Coupled Cluster Doubles F12 Approach.

- Recent Advances in Many-Electron Theory - RAMET- 2017, Goa, India, 9. – 12. 2. 2017
- 57th Sanibel Symposium 2017 (St. Simons Island, GA, USA, 19. – 24. 2. 2017)

PRNOVÁ, Anna - PLŠKO, Alfonz - VALÚCHOVÁ, Jana - KLEMENT, Róbert - GALUSEK, Dušan. Study of thermal behaviour of lanthanum-aluminate glasses by DSC and high temperature XRD analysis. 19. ročníku konference o speciálních anorganických pigmentech a práškových materiálech, 20. 9. 2017, Pardubice, Czech Republic

E. SCHOLTZOVÁ, Problematic Parts of IR Spectrum and Stability of Organoclays - DFT Study. AnalytiX-2017, Fukuoka, Japan, 23. 3. 2017

M. HNATKO, P. ŠAJGALÍK, M. LABUDOVÁ. Silicon nitride - a promising candidate for the bioactive composite implants. 15th International Conference and Exhibition of the European Ceramic Society (ECERS 2017), Budapest, Hungary, 9. – 13. 7 2017

P. ŠAJGALÍK. Silicon nitride-hydroxyapatite bioactive composite. 12th Pacific Rim Conference on Ceramic and Glass Technology Including - Glass and Optical Materials Division Annual Meeting (PACRIM, GOMD 2017), Waikoloa, Hawaii, USA, 21 – 26. 05. 2017

P. ŠAJGALÍK, M. HNATKO, Z. LENČÉŠ, J. DUSZA, P. TATARKO, A. KOVALČÍKOVÁ, M. KAŠIAROVÁ. Thermal shock resistance, wear behaviour and oxidation resistance of silicon nitride based nano-composites. 12th Pacific Rim Conference on Ceramic and Glass Technology Including - Glass and Optical Materials Division Annual Meeting (PACRIM, GOMD 2017), Waikoloa, Hawaii, USA, 21 – 26. 05. 2017

P. ŠAJGALÍK, M. HNATKO, Z. LENČÉŠ, J. DUSZA, P. TATARKO, A. KOVALČÍKOVÁ, M. KAŠIAROVÁ. Thermal shock resistance, wear behavior and oxidation resistance of silicon nitride based nano-composites. 41st International Conference and Exposition on Advanced Ceramics and Composites (ICACC 2017), Hilton Daytona Beach Resort and Ocean Center, Daytona Beach, Florida, USA, 22. – 27. 1. 2017

P. ŠAJGALÍK. Additive-free hot-pressed silicon carbide ceramics: A material with exceptional properties. 41st International Conference and Exposition on Advanced Ceramics and Composites (ICACC 2017), Hilton Daytona Beach Resort and Ocean Center, Daytona Beach, Florida, USA, 22. – 27. 1. 2017

P. ŠAJGALÍK. Role of grain boundary chemistry in silicon nitride based ceramics - experimental and theoretical approach. Modelling and Simulation Meet Innovation in Ceramics Technology (CERMODEL 2017), University of Trento, Italy, 26 – 28. 7. 2017

P. ŠAJGALÍK. Additive-free hot-pressed silicon carbide ceramics - a material with exceptional properties. 10th International Conference on High-performance Ceramics, Nanchang, China, 4. – 7. 7. 2017

P. ŠAJGALÍK. Electrically conductive ceramics - processing and properties. 15th International Conference and Exhibition of the European Ceramic Society (ECERS 2017), Budapest, Hungary, 9 – 13. 7. 2017

P. ŠAJGALÍK, Z. LENČÉŠ, et al. Grain boundary chemistry of silicon nitride based ceramics – Implications to the ceramics properties. In the book of abstracts of the 9th International Symposium on Nitrides (ISNT2017 & ISSNOX5), Hokkiado University, Sapporo, Japan, 27 – 31. 8. 2017

P. ŠAJGALÍK, Z. LENČÉŠ. GB chemistry of silicon nitride based ceramics – Implications to the ceramics properties. In Materials Science and Technology 2017 (MS&T17), Pittsburgh, Pennsylvania, USA, 8 – 12. 10. 2017

P. ŠAJGALÍK, Z. LENČÉŠ, et al. Silicon nitride based ceramics – fantastic diversity of their application. In Francis Cambier symposium: Future perspectives on the magical world of ceramics. Mons, Belgium, 11. – 13. 12. 2017

2018

J. ASHER, An animated visualization of orbital angular momentum and spin-orbit coupling. Conference „MAGIC-2018“, Kragujevac, Serbia, 23. – 28. 09. 2018

J. BUJDÁK, Resonance energy transfer between dye molecules in the colloids of layered nanoparticles. 11th Conference on Colloid Chemistry (Ezsterházy Károly University, Eger, Maďarsko. 27. – 31. 05. 2018

S. KOMOROVSKÝ, Recent advances in the calculation of excitation energies in the framework of fully relativistic TDDFT theory. XIth Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria, 25. 02. – 02. 03. 2018

S. KOMOROVSKÝ, Advances in the calculation of excitation energies in the framework of relativistic four-component TDDFT theory. 7th JCS symposium, Praha, Czech Republic, 21. – 24. 05. 2018

S. KOMOROVSKÝ, Spin−Orbit Heavy Atom on the Light Atom NMR chemical shifts explained. Xth Symposium nuclear magnetic resonance in chemistry, physics and biological sciences, Warszaw, Poland, 26. – 28. 09. 2018

P. ŠAJGALÍK, Z. LENČÉŠ, Role of grain boundary chemistry in silicon nitride based ceramics – Experimental and theoretical approach. 6th International Conference on the Characterisation and Control of Interfaces for High Quality Advanced Materials (ICCCI 2018), Kurashiki, Japan, 9. – 11. 2018

Z. LENČÉŠ, M. RADWAN, A. CZÍMEROVÁ, R. KLEMENT, P. ŠAJGALÍK, R. RIEDEL, Polymer precursor derived silicon oxynitrides and transparent spinel ceramics for LED applications. 12th International Conference on Ceramic Materials and Components for Energy and Environmental Applications (CMCEE 2018), Singapore, 22. – 26. 07. 2018

O. MALKIN, A mystery of a through-space indirect spin-spin coupling between two hydrogen atoms. Conference „Molecules in Extreme Environments, Oslo, Norway, 15. – 17. 01. 2018
O. MALKIN, A mystery of a through-space indirect spin-spin coupling between two hydrogen atoms. Conference „MAGIC-2018“, Kragujevac, Serbia, 23. – 28. 09. 2018
O. MALKIN, A mystery of a through-space indirect spin-spin coupling between two hydrogen atoms, Conference „INSTRUCT ULTRA“ (2nd Structural Bilogy meeting (within H2020), Bratislava, Slovakia, 15 – 16. 11. 2018
V. MALKIN, Visualization of EPR Hyperfine Structure Coupling Pathways. Conference „MAGIC-2018“, Kragujevac, Serbia, 23. – 28. 09. 2018
PRNOVÁ, Anna - VALÚCHOVÁ, Jana - PARCHOVIANSKÝ, Milan - HALADEJOVÁ, Katarína - KLEMENT, Róbert - GALUSEK, Dušan. Preparation and properties of Er- and Nd-doped yttrium-aluminate glasses. Konference o speciálních anorganických pigmentech a práškových materiálech, 19. 9. 2018, Pardubice, Czech Republic

P. ŠAJGALÍK, Si_3N_4-SiC nano-composites sintered with various rare-earth oxide additives for high temperature applications. The Sino-German Symposium, Shangri-la hotel, Xi An, China, 14. – 20. 04. 2018
P. ŠAJGALÍK, Miroslav Hnatko, Zoltán Lenčéš, Jan Dusza, Peter Tatarko Alexandra Kovalčíková, Monika Kašiarová, Thermal shock resistance, wear behavior and oxidation resistance of silicon nitride based nano-composites. ICC7, 7th International Congress on Ceramic, Iguassu Falls, Brasil, 17 – 21. 06. 2018
P. ŠAJGALÍK, New nitrides and carbides for high temperature application. ICC7, 7th International Congress on Ceramic, Iguassu Falls, Brasil, 17 – 21. 06. 2018
P. ŠAJGALÍK, Electrically conductive ceramics - Processing and properties. In ICACC 2018 - 42nd International Conference & Exposition on Advanced Ceramics and Composites, Daytona Beach, Florida, USA, p. 67. 21. – 26. 01. 2018
P. ŠAJGALÍK, Electrically conductive ceramics - processing and properties. In ISAC-6. 6th International Symposium on Advanced Ceramics, Katahira Sakura Hall, Tohoku University, Sendai, Japan, 12. – 14. 03. 2018
P. TATARKO, S. GRASSO, T.G. SAUNDERS, V. CASALEGNO, M. FERRARIS, M.J. REECE, Electric current assisted joining of SiC-based ceramic matrix composites. In ICACC 2018 - 42nd International Conference & Exposition on Advanced Ceramics and Composites, Daytona Beach, Florida, USA, p. 35, 21. – 26. 01. 2018
P. TATARKO, S. GRASSO, Z. CHLUP, T.G. SAUNDERS, V. CASALEGNO, I. DLOUHÝ, M. FERRARIS, M.J. REECE, Field Assisted Joining of Monolithic CVD-SiC Materials and Ceramic Matrix Composites. In CMCEE-12. 12th International Conference on Ceramic Materials and Components for Energy and Environmental Applications, Suntec Convention & Exhibition Centre Singapore, Singapore, 22. – 27. 07. 2018
P. TATARKO, S. GRASSO, Z. CHLUP, T.G. SAUNDERS, V. CASALEGNO, I. DLOUHÝ, M. FERRARIS, M.J. REECE, Electric current assisted solid-state diffusion bonding of SiC and CMCs. In 1st International Workshop on Advanced SiC-based Ceramic Processing and Joining, Ningbo Institute of Materials Technology and Engineering (NIMTE), Chinese Academy of Sciences, Ningbo, China, 27. 06. 2018

2019

BOČA M. – ŠIMURDA M. – ŠVEC P. - ŠVEC P. Jr. – JANIČKOVIČ D. – CZÍMEROVÁ A. – KUBÍKOVÁ B. –MLYNÁRIKOVÁ J. Unusual phase transformations in ternary fluoride systems. In 19th European Symposium on Fluorine Chemistry (19th ESFC), 25-31 August 2019, Warsaw Poland.

BUJDÁK J. The phenomena occurring in the systems of layered silicates and organic dyes. Research Work and Collaboration Symposium: Molecules and Materials for Life, Topic: Interaction of Inorganic Clusters, Cages, and Containers with Light, Villa Lanna Prague, Czech Republic, 19. 3. 2019

BUJDÁK J. Energy transfer between dye molecules in the hybrid materials with layered silicates. Research Work and Collaboration Symposium: Molecules and Materials for Life, Topica: Interaction of Inorganic Clusters, Cages, and Containers with Light, Liblice, Czech Republic, 5. 12. 2019.

GALUSEK D. High temperature corrosion and oxidation of advanced ceramics and glass-ceramic composites; Fefra Pragueat, The Czech Association of Technical Societies at Novotného Lávka 5, Prague, Czech Republic, 24 – 26. 4. 2019

GALUSEK D. FunGlass Centre: progress of a successful international Centre in the field of functional glasses; 93rd Annual Meeting of the German Society of Glass Technology (DGG) in conjunction with the French Union for Science and Glass Technology (USTV) Annual Meeting, Nürnberg, Germany, 13. - 15. May 2019

KOMOROVSKÝ S. - CHERRY P. - REPISKÝ M. Relativistic theory for prediction of excitation energies of both closed- and open-shell species. In CESTC 2019. 17th Central European Symposium on Theoretical Chemistry, Burg Schlaining, Austria, 9. – 12. 9 2019,

MALKIN O. Indirect NMR spin-spin couplings between atoms possessing lone pairs and between two hydrogen atoms: Can we learn from the latter about the former? Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria, 11. - 15. 3 2019

MALKIN O. A mistery of a through-space indirect spin-spin coupling between two hydrogen atoms“, 19th deMon developers workshop, Frejus, France, 26. – 30. 5. 2019

MALKIN V. – MALKIN O, Visualization of EPR hyperfine structure coupling pathways, 19th deMon developers workshop, Frejus, France, 26. – 30. 5. 2019

MALKIN V. Calculations and interpretation of the EPR parameters in the framework of 2- and 4-component DFT approach, XIth EFEPR Conference (EF EPR 2019), Bratislava, 1. – 5. 9. 2019

PRNOVÁ A. – VALÚCHOVÁ J. – DOHNALOVÁ Ž. – HANZEL O. – KLEMENT R. – BRUNEEL E. – GALUSEK D. Preparation of Al2O3-Y2O3 glass microspheres; influence of particle size distribution on thermal behavior of prepared systems., Konference o speciálních anorganických pigmentech a práškových materiálech, Pardubice, Czech Republic, 18. 9 2019

SCHOLTZOVÁ E. - JANKOVIČ Ľ. - ŠKORŇA P. - MORENO RODRÍGUEZ D. - TUNEGA D. Insight into the stability of beidellite intercalates. In BIT´s 7th Annual Conference of AnalytiX-2019, Singapore, Exploring Innovative Advances and Applications, 12. – 14. 4. 2019

ŠAJGALÍK P. Porous silicon nitride: A material for the bioactive composite implants. In ICACC 2019. 43rd International Conference & Exposition on Advanced Ceramics and Composites, Daytona Beach, Florida, USA, 27. 1. – 1. 2. 2019

ŠAJGALÍK P. - HNATKO M. - KAŠIAROVÁ M. - SEDLÁČEK J. - BYSTRICKÝ R. - LENČÉŠ Z. - GALUSKOVÁ D. Corrosion of silicon nitride and alumina based ceramics by molten iron. REFRA PRAGUE 2019, Prague, Czech Republic

ŠAJGALÍK P. New nitrides and carbides for high temperature application. In ICCT. 7th International Conference on Chemical Technology, Mikulov, Czech Republic, 15. – 17. 4. 2019,

ŠAJGALÍK P. - SEDLÁČEK J. - KOVALČÍKOVÁ A. - HAN X. - ZHANG C. Ultra-high creep resistant silicon carbide ceramics. In XVI ECerS Conference, Torino, Italy, 16. – 20. 6. 2019

ŠAJGALÍK P. Ceramic research in Slovakia: potential for R&D cooperation. In CICC-11: The 11th International Conference on High-Performance Ceramics, Kunming, China, 25. – 29. 5. 2019

TATARKO P. Development of ultra-high temperature ceramics by field assisted sintering technology, 5th Conference of The Serbian Society for Ceramic Materials, Belgrade, Serbia, 11. – 13. 6. 2019

2020

ASHER J. – HRICOVINI M. – HRICOVINI M. Photochemical properties of quinazolinone- derivative Schiff's bases: Anti-syn isomerisation across the N-N bond. In XIIIth Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria, 1. – 6. 3. 2020.

BOHÁČ, P. – CZÍMEROVÁ, A. – SASAI, R. – BUJDÁK, J. Photophysical properties of hybrid systems based on layered silicates and cyanine dyes. In ICMS-2020. 3rd International Conference on Material Science, Tripura University, India, 4. – 6. 3. 2020

KOMOROVSKÝ, S. Relativistic DFT calculations of spectroscopic parameters for paramagnetic species: theoretical and practical considerations. In XIIIth Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria, 1. – 6. 3. 2020

LENČÉŠ Z. - RADWAN M. – PETRISKOVÁ P. – CZÍMEROVÁ A. – ŠAJGALÍK P. Transparent/translucent $MgAl_2O_4$ and MgAlON-based phosphors for solid state lighting and

photocatalytic applications. In 44th International Conference & Exposition on Advanced Ceramics & Composites, Daytona Beach, Florida, USA, 26 – 31. 1. 2020

MALKIN O. L. – KOMOROVSKY S. – MALKIN V. G. Beyond the Dirac vector model: why one-bond NMR spin-spin coupling can be negative. In XIIIth Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria, 1. – 6. 3. 2020.

BUJDÁK, J. Resonance energy transfer in hybrid systems of layered nanoparticles and laser dyes.

- ICMS-2020. 3rd International Conference on Material Science, 4. – 6. marec 2020, Tripura University, India, 6. 3. 2020
- Recent Trends in Condensed Matter Physics, School of Physical Sciences, Indian Association for the Cultivation of Science, 2. – 3. 3. 2020, CV Raman Hall, IACS, Kolkata, 2. 3. 2020

2021

BOČA, M. - KUBÍKOVÁ, B. - NETRIOVÁ, Z. - MATSELKO, O. - MLYNÁRIKOVÁ, J. Systematic research on ternary fluoride systems based on selected lanthanides. In International conference MELTS, Ekaterinburg, Russia, 12. – 18. 9. 2021 (online)

KOMOROVSKÝ, S. Prediction of spectroscopic parameters for paramagnetic species containing heavy elements: Can the relativistic DFT methods do the job? Workshop Paramagnetic NMR in f elements, Toulouse, France, 21. – 24. 11. 2021

PÁLKOVÁ H. Infrared spectroscopy as powerful tool to study clay minerals subjected to various types of modification, NanoOstrava 2021, Ostrava, Czech Republic, 17. – 20. 05. 2021 (online)

PRNOVÁ, A - PLŠKO, A. - VALÚCHOVÁ, J. - PECUŠOVÁ, B. - MAJEROVÁ, M. - KLEMENT, R. - GALUSEK, D. Termická analýza hlinitanových skiel. Konference o speciálních anorganických pigmentech a práškových materiálech, Pardubice, Czech Republic, 23. 9. 2021

TATARKO P. Joining and integration of silicon carbide based ceramics. The 14th Conference for Young Scientists in Ceramics, Novi Sad, Serbia, 20. – 23. 10. 2021

TATARKO P. Joining of SiC-based advanced ceramics. YCN Webinar Series, Young Ceramists Network, ECERS, https://www.youtube.com/watch?v=w629cDUEsHo 19. 01. 2021

Invited lectures at institutions abroad

2016

J. ASHER: Visualisation of the 3D g-tensor density", Technical University of Munich, Germany, 8. 8. 2016

M. BOČA: Corrosion behaviour of Different Construction Materials in FLiNaK with Addition of Fluorides Salts Based on Elements of Corroded Materials,

- University of Science and Technology, Beijing, China, 9. 5. 2016
- Shanghai Institute of Applied Physics, Chinese Academy of Science, Shanghai, China, 14. 5. 2016
- Northeastern University, Shenyang, China, 16. 5. 2016

J. BUJDÁK: Hybrid systems based on organic dyes and layered silicates: Fundamentals and potential applications, Faculty of Sciences, Bilbao University, Spain, 18. 07. 2016

D. GALUSEK: Visible Broadband Luminescence of Transition Metals Doped Aluminate and Aluminosilicate Glass and Glass-Ceramics, School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an, China, 14. 12. 2016

B. KUBÍKOVÁ: Critical Evaluation of Volume Properties of Molten Fluoride Salts.

- Shanghai Institute of Applied Physics, Chinese Academy of Science, Shanghai, China, 15. 5. 2016
- Notheastern University, Shenyang, China, 16. 5. 2016

O. MALKIN: Is there anything interesting about the DSO contribution to NMR spin-spin couplings?, CTCC Tromsø, Norway, 12. 8. 2016

V. MALKIN: Calculations of the EPR g-tensor in the framework of two- and four-component HF and DFT approaches, CTCC Tromsø, Norway, 12. 8. 2016

V. MALKIN: Visualization of EPR hyperfine coupling pathways, Technical University of Berlin, Germany, 7. 12. 2016

N.S. PATEL: High-temperature properties of materials corrosion in molten salts. Solar Thermal Group, Australian National University, Canberra, Australia, 9. 12. 2016

P. ŠAJGALÍK: Sintering, Northwestern Polytechnical University, Xi An, China

- Sintering, 29. 12. 2016
- Thermal shock resistance, wear behavior and oxidation resistance of silicon nitride based nano-composites, 29. 12. 2016

2017

M. BOČA, Molten salts: from fundamental research to hydrogen economy, Shanghai Institute of Applied Physics, Chinese Academy of Science, Šanghaj, China, 23.05.2017

M. BOČA, XPS and NMR spectroscopy of ternary fluorides.

- Shanghai Institute of Applied Physics, Chinese Academy of Science, Šanghaj, China, 23.05.2017
- Northeastern University, Shenyang, China, 25.05.2017

T. BUČKO, Enthalpy, entropy, and confinement: a DFT modelling beyond static approach, seminár, IFP Energies nouvelles (IFPEN) Lyon, France, 13. 9. 2017

J. BUJDÁK, Hybrid materials based on organic dyes and layered silicates: Fundamentals and potential applications. Department of Chemistry, Jamia Millia Islamia, New Delhi, India, 21.2. 2017

S. KOMOROVSKÝ, Development of open-shell TDDFT method within four-component domain in ReSpect program, Helmholtz-Zentrum Dresden-Rossendorf: Chemistry of the f-elements, Dresden, Germany, 6. 6. 2017

S. KOMOROVSKÝ, Recent advances in the calculation of excitation energies in the framework of fully relativistic TDDFT theory, Technische Universität Berlin, Institut für Chemie, Berlin, Germany, 8. 9. 2017

M. KORENKO, Molten Fluoride Science in Slovakia, Wisconsin University Madison, Madison, USA 23.3. 2017

M. KORENKO, Solar Thermal Electrolysis of Mg from molten Fluorides, Institute of High Energy Physics, Čínska Akadémia Vied, Beijing, China, 24.8. 2017

B. KUBÍKOVÁ, J. MLYNÁRIKOVÁ, E. MIKŠÍKOVÁ, M. ŠIMURDA, M. BOČA, Physico-chemical properties of molten systems based on lanthanum fluoride,

- Shanghai Institute of Applied Physics, Chinese Academy of Science, Shanghai, China, 23.05.2017
- Northeastern University, Shenyang, China, 25.05.2017

B. KUBÍKOVÁ, J. MLYNÁRIKOVÁ, M. BOČA, Physico-chemical investigation of potassium cryolite molten systems, Northeastern University, Shenyang, China, 25.05.2017

O. MALKIN, Beyond numbers: visualization of properties, Paris Lodron University of Salzburg, Austria, 8.9.2017

O. MALKIN, “A mystery of a through-space indirect NMR spin-spin coupling between two hydrogen atoms”, Fukui Institute for Fundamental Chemistry, Kyoto, Japan, 11.12.2017.

O. MALKIN, A mystery of a through-space indirect NMR spin-spin coupling between two hydrogen atoms, Nagoya University, Japan, 13.12.2017

V. MALKIN, Calculations of NMR and EPR parameters, Paris Lodron University of Salzburg, Austria, 8.9.2017

V. MALKIN, Relativistic calculations of EPR parameters and their interpretation, Fukui Institute for Fundamental Chemistry, Kyoto, Japan, 11.12.2017

V. MALKIN, Calculations of NMR and EPR parameters, Paris Lodron University of Salzburg, 8.9.2017

V. MALKIN, Relativistic calculations of EPR parameters and their interpretation, Nagoya university,

Japan, 13.12.2017

J. Noga, Optimized Thouless expansion- an alternative to orbital optimization methods. Indian Institute of Technology (IIT), Mumbai, India, 13.2. 2017

P. TATARKO, Introduction to PhD"; The 4th Yokohama National University (YNU) Symposium, 01.10.-02.10.2017, Maholova Minds Miura, Japan

2018

T. BUČKO, On the origin of the difference between type A and type B skeletal isomerization of C7 alkenes: an ab initio MD study, Karlsruhe Institute of Technology, Karlsruhe, Germany, 19. 11. 2018

J. BUJDÁK, Resonance energy transfer and other photophysical phenomena occurring in the hybrid systems of layered silicates and organic dyes, National Institute for Materials Science, Tsukuba, Japan, 08. 06. 2018

M. KORENKO, Solar thermal production og Mg from MgO, Institute of High Temperature Physics, Chinese Academy of Sciences, Beijing, China, 06. 07. 2018

O. MALKIN, A mystery of a through-space indirect spin-spin coupling between two hydrogen atoms. The Paris Lodron University of Salzburg, Austria, 7. 09. 2018

V. PAVLÍK, M. BOČA, Electrochemical investigation of the molten systems containing rare earth metals. Tananaev Institute of Chemistry and Technology of Rate Elements and Mineral Raw Materials, Kola Science Centre of the Russian Academy of Sciences, Apatity, Russia, 26. 09. 2018

V. PAVLÍK, M. BOČA, Physico-chemical and electrochemical properties of a new type of ionic liquids – deep eutectic solvents, Ukrainian State University of Chemical Technology, Dnipro, Ukraine, 09. 10. 2018

P. ŠAJGALÍK, Silicon nitride based ceramics – fantastic diversity of their application, Northwestern Polytechnic University, Xi An, China, 19. 11. 2018

P. TATARKO, Mechanical properties of ceramics, Ningbo Institute of Materials Technology and Engineering (NIMTE), Chinese Academy of Sciences, Ningbo, China, 29. 06. 2018

2019

BARLOG M. – PÁLKOVÁ H. – BUJDÁK J. Spectral properties of hybrid sytems based on organomodified clay minerals and Rhodamine 6G, Center for Materials Nanoarchitectonics (WPI-MANA) at the National Institute for Materials Science (NIMS), Tsukuba, Japan, 18. 07. 2019.

BOČA M. Spectroscopy, séria prednášok, School of Metallurgy, Northeastern University, Shenyang, China, 8. - 25. 10. 2019

BUJDÁK J. Photophysical phenomena occurring in hybrids of expandable phyllosilicates and organic dyes. Bayreuth, Univerzity of Bayreuth, Germany, 25. 01. 2019

HANZEL O. – LENČÉŠL Z. – KIM I.-W. – ŠAJGALÍK P. Preparation of SiC-graphene composites with high functional properties, Northwestern Polytechnical University, Xi'an, China, 31. 05. 2019

CHROMČÍKOVÁ M. – HRUŠKA B. – LIŠKA M. Acquisition of valuable data by analysis of unsuccessful thermodilatometric experiments. Thermoanalytical seminar, Brno, Czech Republic, 10. 11. 2019

KORENKO M. Molten Salts Chemistry in Slovakia, School of Metallurgy, Northeastern University, Shenyang China, 6. 09. 2019

KUBÍKOVÁ B. Phase equilibrium of condensed systems, School of Metallurgy, Northeastern University, Shenyang, China, 8. 10. 2019

KUBÍKOVÁ B. Density and volume properties of molten systems. Fluoride molten systems: results and comparison, School of Metallurgy, Northeastern University, Shenyang, China, 9. 10. 2019

MALKIN O. – KOMOROVSKÝ S. – MALKIN V. Beyond the Dirac vector model?, Technical University Berlin, Germany, 3. 12 2019

PRNOVÁ A. – VALÚCHOVÁ J. – PARCHOVIANSKY M. – KLEMENT R. – GALUSEK D. HP sintering of yttrium aluminate glasses, impact of particle size on mechanical properties, University of Ghent, Belgium

TATARKO P. Development and Joining of Advanced Ceramics for Extreme Applications using Field Assisted Technology, Northwestern Polytechnical University, Xi'an, China, 3. 05. 2019

TATARKO P. Field assisted processing for the development and joining of ceramics for extreme

environments, Ningbo Institute of Materials Technology and Engineering (NIMTE), Chinese Academy of Sciences, Ningbo, China, 8. 11. 2019

2021

PRNOVÁ, A. - PLŠKO, A. - VALÚCHOVÁ, J. - PECUŠOVÁ, B. - MAJEROVÁ, M. - KLEMENT, R. - GALUSEK, D. Thermal analysis of aluminium glases, University of Pardubice, Pardubice, Czech Republic, 23. 9. 2021

2.3.8. List of researchers who served as members of the organising and/or programme committees

M. Boča
- The Solid State Chemistry Conference (SSC 2016), 18. - .23. 09. 2016, Prague, Czech Republic, Programe Committee and Advisory Board
- Nano Ostrava 2017, 22.-25. 05. 2017, Ostrava, Czech Republic, Scientific Committee
- Nano Ostrava 2019, 13. -16. 05. 2019, Ostrava, Czech Republic, Scientific Committee
- Nano Ostrava 2021, 17. -20. 05. 2021, Ostrava, Czech Republic, Scientific Committee
- 11th international symposium on Molten Salts Chemistry and Technology, 19. – 23. 2019, Orleáns, France, International Advisory Board
- 19th European Symposium on Fluorine Chemistry, 25. – 31. 08. 2019, Warszaw, Poland, International Advisory Board
- International Conference „MELTS", 12. – 18. 09. 2021, Yekaterinburg, Russia, International Committee

J. Bujdák
- 8th Mid-European Clay Conference MECC2016, 4. – 8. 7. 2016, Košice, Slovak Republic
- 3rd International Conference on Applied Mineralogy & Advanced Materials, 23. – 27.7. 2018, Polytechnic University of Bari, Bari, Italy,
- 11th Conference on Colloid Chemistry, 28. – 30. 5. 2018, Ezsterházy Károly University, Eger, Hungary

D. Galusek
- Joint meeting DGG-USTV, 13 – 15 May 2019, Nürnberg, Germany
- Engineering Ceramics 2019, 12. – 16. May 2019 Smolenice, Slovak Republic
- 14th International Conference on Solid State Chemistry, June 14-17, 2021, Trenčín, Slovak Republic

O. Hanzel
- Processing and properties of advanced ceramics and glasses, 20. -22. 11. 2019, Ráztočno, Slovak Republic

M. Hnatko
- Processing and properties of advanced ceramics and glasses, 20. -22. 11. 2019, Ráztočno, Slovak Republic

S. Komorovský
- Workshop on Modern Methods in Quantum Chemistry, 2020, Mariapfarr
- Paramagnetic NMR in f elements, Toulouse, France, 2021

B. Kubíková
- 9th Workshop: Interactions of melts with progressive inorganic materials, 15.-16.10.2018, Borinka, Slovak Republic

V. Kureková

- 5th Workshop of Slovak Clay Group Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology, 21. - 23. 05.2018, Banská Štiavnica, Slovakia

Z. Lenčéš
- ECerS 2017 - 15th Conference & Exhibition of the European Ceramic Society, 9. - 13. 7. 2017 Budapest, Hungary
- Engineering Ceramics 2019, 12. – 16. May 2019 Smolenice, Slovak Republic

J. Madejová
- 8th Mid-European Clay Conference MECC2016, 4. – 8. 7. 2016, Košice, Slovak Republic
- 5th Workshop of Slovak Clay Group Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology, 21. - 23. 05.2018, Banská Štiavnica, Slovakia
- EUROCLAY 2019, 1. - 5. July 2019, Paris, France

O. Malkin
- XIIIth Workshop on Modern Methods in Quantum Chemistry, 1. – 6. 3. 2020, Mariapfarr, Austria
- XIVth Workshop on Modern Methods in Quantum Chemistry, 6. – 11. 3. 2021, Bratislava, online

V. Malkin
- 9th Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria,
- 23. - 28. 02. 2016
- Xth Workshop on Modern Methods in Quantum Chemistry, 5. – 10. 3. 2017, Mariapfarr, Austria
- 11th Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria, 25. 2. - 02. 3. 2018
- XIIth Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Austria 2019
- XIIIth Workshop on Modern Methods in Quantum Chemistry, 1. – 6. 3. 2020, Mariapfarr, Austria

H. Pálková
- 5th Workshop of Slovak Clay Group Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology, 21. - 23. 05.2018, Banská Štiavnica, Slovakia
- 8th Mid-European Clay Conference MECC2016, 4. – 8. 7. 2016, Košice, Slovak Republic

E. Scholtzová
- 8th Mid-European Clay Conference MECC2016, 4. – 8. 7. 2016, Košice, Slovak Republic

P. Šajgalík
- The Solid State Chemistry Conference (SSC 2016), 18. - .23. 09. 2016, Prague, Czech Republic
- 6th International Congress on Ceramics – From Lab to Fab, 21. – 25. 8. 2016, Dresden, Germany
- 91st DKG Annual Meeting and Symposium on High-Performance Ceramics, 9. – 7. 3. 2016, Freiberg, Germany
- 4th International Symposium on New Frontier of Advanced Si-based Ceramics and Composites (ISASC 2016), 25. – 28. 9. 2016, Busan, Korea
- 40th International Conference and Exposition on Advanced Ceramics and Composites, 24. – 29. 1. 2016, Daytona Beach, Florida, USA, 2016
- PACRIM 2017 12th Pacific Rim Conference on Ceramic and Glass Technology, 21 – 26 May 2017, Hawai, USA
- 9th International Symposium on Nitrides (ISNT2017 & ISSNOX5), August 27 - 31, 2017, Hokkiado University, Sapporo, Japan
- 41st International Conference and Exposition on Advanced Ceramics and Composites (ICACC) Daytona Beach, Florida, USA
- 15th International Conference and Exhibition of the European Ceramic Society (ECERS 2017), 9. – 13. 2017, Budapest, Hungary

- 12th International Conference on Ceramic Materials and Components for Energy and Environmental Applications, Suntec Convention & Exhibition Centre Singapore, 22. – 27. 07. 2018, Singapore,
- 44th International Conference & Exposition on Advanced Ceramics & Composites, 26 – 31. 1. 2020 Daytona Beach, Florida, USA

F. Šimko
- Interactions of melts with progressive inorganic materials, 15.10.-16.10.2018, Borinka, Slovak Republic

P. Tatarko
- 5th Conference of The Serbian Society for Ceramic Materials, 11. - 13. 6. 2019, Belgrade, Serbia
- HT-CMC/10th, Symposium – Conference Topic 13: Joining, 22 – 26. 9. 2019, Bordeaux, France
- XVI ECerS Conference 2019, Symposium: HT Processes and Advanced Sintering, 16. – 20. 6. 2019, Torino, Italy
- 44th International Conference & Exposition on Advanced Ceramics & Composites, 26 – 31. 1. 2020 Daytona Beach, Florida, USA

J. Valúchová
- 8th Mid-European Clay Conference MECC2016, 4. – 8. 7. 2016, Košice, Slovak Republic

a) Long term stays as post-doc or in position of visiting researchers. The list of the stays longer than 3 months is below.

Peter Boháč
Karlsruhe Institute of Technology, Germany, 1. 11. 2017 – 6. 6. 2019
Sandwich-VP project financed by the German Federal Ministry of Economic Affairs and Energy under contract 02E11587A, The project focuses on the study of barrier materials for underground nuclear waste deposits.

Marián Matejdes
Yamaguchi University, Japan, 8. 6. 2015 – 7. 6. 2017, JSPS Fellowship Programs for Overseas Researches, ID No. P15742, Title of project: Photofunctionalities of nanosheets and nanosheet based materials: tuning their optical properties. The project is aimed at studying the synthesis of hybrid materials with switchable optical properties.

Stanislav Kedžuch
The main goal of the visit was cooperation in the development of methods with explicit incorporation of electron correlation. The F12-C method was implemented within the Gellan package developed by the Japanese partner. Integrals for the use of the F12-C method in perturbation theory were also implemented. The three-electron integrals required for full implementation of F12 method were prepared.
Kobe University, Japan / 5. 9. 2016 – 15. 1. 2017

Michal Korenko
Engineering College, Valparaiso University, Valparaiso, Indiana, USA, 04/2014 – 12/2016
Postdoctoral fellowship within ARPA-E project / US Department of Energy, cooperative agreement DE– AR0000421, the project was focused on the development and commercialization of high temperature solar thermal electrolysis of MgO for Mg production. Magnesium is produced by electrolysis directly from the MgO dissolved in the fluoride electrolyte. Part of the energy required for high-temperature electrolysis is supplied by solar heat in a parabolic solar reactor, which allows the integration of both primary electrolysis and in situ magnesium refining. The ultimate goal of the project is a new, ecologically- and economically-competitive technology that could disrupt the dominance of energy-intensive Pidgen process, which is currently the predominant industrial method for producing Mg.

Marián Kucharík
Primary Metal Technology (PMT) - Technology development, Hydro Aluminium j.s.c. Årdal, Norway, projektový inžinier (11/2008 – 08/2016). Research and development of aluminum production technology by the Hall-Heroult process.

Martin Pentrák
Department of Natural Resources and Environmental Sciences, University of Illinois at Urbana-Champaign, USA, Postdoctoral Research Associate, 06/2012 – 09/2016,
Title of project: Research and development of new progressive nanocomposites based on organo-modified clay minerals suitable for environmental and industrial applications.

Anna Prnová
X-ray science division, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, USA, Fulbright grant 15-22-08, 11/2015 – 03/2016, Structure of solids and liquids in the Y_2O_3-Fe_2O_3 and Y_2O_3-Ga_2O_3 systems by high energy X-ray diffraction and by Mőssbauer spectroscopy.

2.3.9. List of researchers who received an international scientific award

2016

Boháč Peter
Best student oral presentation
Granted by: Organizing committee of Mid-European Clay Conference (4. - 8. 7. 2016), Košice, Slovakia
Description: Award for the best student presentation at an international conference (29 countries).

Šajgalík Pavol
Lee Hsun Lecture Award
Granted by: Institute of Metals Research, Chinese Academy of Sciences, Shenyang, China
Description: For his outstanding contribution to the materials science and engineering.

2018
Komorovský Stanislav
Petr Sedmer Award
Granted by: Jan Marek Marci Spectroscopic Society, Czech Republic
Description: For the best published work in the field of nuclear magnetic resonance. Award delivered in 2018 was for publication in J. Am. Chem. Soc. 138, 8432–8445 (2016).

Lenčéš Zoltán
Prize for International Cooperation
Granted by: Polish Ceramic Society in Description: Krakow, 10.9.2018

2019
Liška Marek
Silver medal
Granted by: University of Pardubice
Description: For merits and for long-term cooperation in the field of science and research

Liška Marek
Memorial medal
Granted by: University of Pardubice
Description: vote of thanks for long-term cooperation

- **Position of individual researchers in the national context**

2.3.10. List of invited/keynote presentations at national conferences, as documented by programme or invitation letter

2016

P. BOHÁČ: Study of energy transfer between cationic dyes on thin layered films of clay minerals. Workshop: UV-Vis-NIR Spectrophotometry in Materials Research, Bratislava, 21. 1. 2016

J. BUJDÁK: Applications of UV-VIS spectroscopy: Hybrid systems of clay minerals and organic dyes. Workshop: UV-Vis-NIR Spectrophotometry in Materials Research, Bratislava, 21. 1. 2016

A. ČEKLOVSKÝ: Optical properties of hybrid nanomaterials. Workshop: UV-Vis-NIR Spectrophotometry in Materials Research, Bratislava, 21. 1. 2016

2017

P. BOHÁČ, Influence of temperature on absorption spectra of hybrid systems of layered silicates with organic dyes. Workshop: Applications in UV-Vis-NIR spectrophotometry, Bratislava, 26. 9. 2017

P. BOHÁČ, Influence of temperature on photophysical properties of materials. Possibilities of using UV-VIS-NIR spectroscopy, Seminar HERMES, Košice, 3.10.2017, Bratislava 5.10.2017

J. BUJDÁK, Dye metachromasy for detection and characterization of clay minerals. 4. Workshop of Slovak National Clay Group, Stará Lesná, 19. 6. 2017

J. BUJDÁK, Dye metachromasy for detection and characterization of colloidal layered silicate particles. Workshop: UV-Vis-NIR Spectrophotometry in Materials Research, Bratislava, 26. 9. 2017

A. ČEKLOVSKÝ, Spectral behaviour of TMPyP/layered silicate hybrid nanomaterials in aqueous dispersions of reduced-charge montmorillonites. Workshop: UV-Vis-NIR Spectrophotometry in Materials Research, Bratislava, 26. 9. 2017

S. KOMOROVSKÝ, Moving relativistic quantum chemistry out of the shadow: Relativistic paramagnetic NMR, SASPRO seminar, Bratislava, 7. 2. 2017

2018

J. BUJDÁK, Hybrid materials based on layered nanoparticles and photoactive organic dyes, Univerzita J. Selyeho, Komárno, Slovakia, 5. 11. 2018

J. BUJDÁK, Chemometry for data processing in natural sciences. What's new in microbiology? Mikulášska chata, Demänovská dolina, Nízke Tatry, Slovakia, 14. – 18. 03. 2018

S. KOMOROVSKÝ, Simple trick in the MO analysis of spectroscopic properties. GOLDCAT workshop, Smolenice, Slovakia, 22. – 24. 11. 2018

2019

ASHER J. Photochemical properties of potential anticancer agents: Anti-syn isomerization of 2,3-disubstituted quinazolinones, INSTRUCT ULTRA, 3rd Structural Biology Meeting, Bratislava, Hotel Tatra, Slovakia, 14. – 15. 11. 2019

MALKIN, V. - MALKIN, O. Calculations and interpretation of the EPR parameters in the framework of 2- and 4-component DFT approach. In XIth EFEPR 2019 Conference: Book of abstracts. Bratislava: Publisher SCHK, 2019.

2.3.11. List of researchers who served as members of organising and programme committees of national conferences

Bujdák Juraj

– 7th Workshop of Slovak Clay Group: Clay Minerals and Selected Industrial Minerals in Material Science, Applications and Environmental Technology, 7. 9. 9. 2020, Demänovská dolina, Slovakia,

- 8th Workshop of Slovak Clay Group. Clay Minerals and Selected Industrial Minerals in Material Science, Applications and Environmental Technology, 6. – 8. 9. 2021, Habovka, Slovakia

Galusek Dušan
- Processing and properties of advanced ceramics and glass including
- Joint annual meeting of the Silicate Scientific-Technological Society & SKLOKERAM Conference, Osrblie, 13.-15. October 2021

Madejová Jana
- Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology, 19. - 21. 6. 2017, Stará Lesná, Slovakia
- 6th Workshop of Slovak Clay Group: Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology, 27. – 28. 5. 2019, Banská Bystrica, Slovakia
- 7th Workshop of Slovak Clay Group: Clay Minerals and Selected Industrial Minerals in Material Science, Applications and Environmental Technology, 7. 9. 9. 2020, Demänovská dolina, Slovakia,
- 8th Workshop of Slovak Clay Group. Clay Minerals and Selected Industrial Minerals in Material Science, Applications and Environmental Technology, 6. – 8. 9. 2021, Habovka, Slovakia

Pálková Helena
- Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology, 19. - 21. 6. 2017, Stará Lesná, Slovakia
- 6th Workshop of Slovak Clay Group: Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology, 27. – 28. 5. 2019, Banská Bystrica, Slovakia
- 7th Workshop of Slovak Clay Group: Clay Minerals and Selected Industrial Minerals in Material Science, Applications and Environmental Technology, 7. 9. 9. 2020, Demänovská dolina, Slovakia,
- 8th Workshop of Slovak Clay Group. Clay Minerals and Selected Industrial Minerals in Material Science, Applications and Environmental Technology, 6. – 8. 9. 2021, Habovka, Slovakia

T. Šimonová
- 8th Workshop of Slovak Clay Group. Clay Minerals and Selected Industrial Minerals in Material Science, Applications and Environmental Technology, 6. – 8. 9. 2021, Habovka, Slovakia

2.3.12. List of researchers who received a national scientific award

2016

Madejová Jana: Medal of the Slovak Academy of Sciences for support of science, conferred by the Presidium of Slovak Academy of Sciences
Malkin Oľga: Medal of the Slovak Academy of Sciences for support of science, conferred by the Presidium of Slovak Academy of Sciences
Malkin Vladimír: Medal of the Slovak Academy of Sciences for support of science, conferred by the Presidium of Slovak Academy of Sciences

2017

Belušáková Silvia: Won 1st place in the Slovak Spectroscopic Society's Competition of young spectroscopists for work in the field of the application of spectroscopic methods in the description of Förster resonance energy transfer in hybrid nanomaterials based on layered silicates and organic laser dyes.
Boháč Peter: Won 3rd place in the Slovak Spectroscopic Society's Competition of young spectroscopists for work in the field of the application of spectroscopic methods in the evaluation of photophysical properties of hybrid materials based on cyanine dyes and layered silicates.

Madejová Jana:

- Award for authors of excellent publications (category: highly-cited publications), granted by the Presidium of Slovak Academy of Sciences
  Description: Publications which were highly cited during the years 2013 - 2015, which are also classified as "Highly Cited Papers" according to the parameters of the database Essential Science Indicators Web of Science. The number of citations is standardized for the average citation rate in a given scientific field. Publication: MADEJOVÁ, J. FTIR techniques in clay mineral studies. In Vibrational Spectroscopy, 2003, vol. 31, p. 1-10 (682 citations)
- Nominee of the survey SLOVENKA ROKA 2018 ("Slovak Woman of the Year 2018") in the category Research and Science and Research, conferred by the weekly magazine Slovenska, Slovak Television RTVS, and the Slovak National Theater. Description: The philosophy of the survey is to acknowledge women who are successful in their field of interest.

Noga Jozef: Award for authors of excellent publications (category: highly-cited publications), granted by the Presidium of Slovak Academy of Sciences
Description: Publications which were highly cited during the years 2013 - 2015, which are also classified as "Highly Cited Papers" according to the parameters of the database Essential Science Indicators Web of Science. The number of citations is standardized for the average citation rate in a given scientific field. Publication: HELGAKER, T. – KLOPPER, W. – KOCH, H. – NOGA, J. Basis-set convergence of correlated calculations on water. In Journal of Chemical Physics, 1997, vol. 106, no. 23, p. 9639-9646 (1386 citations)

2019

Galusek Dušan: Award of the Minister of Education of Science, Research and Sports of the Slovak Republic for science and technology, granted by: Ministry of Education, Science and Research of the Slovak Republic (8. 11. 2019)
Description: Research team of the year, team leader
Hanzel Ondrej: Competition of young scientists of SAS, 2nd place within Scientific Section II: Life, Chemical, Medical, and Environmental Sciences, conferred by the Presidium of Slovak Academy of Sciences
Description: For a series of papers on the topic "Electro-discharge machining of ceramic-carbon nanostructure composites".
Malkin Oľga: Award for the authors of an excellent publication, M. Dračínský, M. Buchta, M. Buděšínský, J. Vacek-Chocholoušová, O. L. Malkin, I. Stará and I. Starý, Dihydrogen contacts observed by through-space indirect NMR coupling, Chem. Sci. 9 (2018), 7437-7446. Conferred by the Presidium of Slovak Academy of Sciences.

2020

Galusek Dušan: Scientist of the year, granted by: Slovak Centre of Scientific and Technical Information, Slovak Academy of Sciences, Association of Slovak Scientific and Technical Societies ZSVTS, Description: Award in the category „Personality of international scientific and technical cooperation"

2021

Boháč Peter: Honorable mention for the Competition of Young Scientists of the Slovak Academy of Sciences, granted by: The Presidency of the Slovak Academy of Sciences
Description: For the paper Photophysical properties of hybrid systems based on layered silicates and cyanine dyes, 26.4.2021
Komorovský Stanislav: The award of the Presidency of the Slovak Academy of Sciences for the top publication in the category of „Publications with the highest impact factor acording to SJR", granted by the Presidency of the Slovak Academy of Sciences
Description: the authors formulated a new fundamental law that illuminates the effect of a heavy atom on the NMR shift of a neighbouring light atom.. VÍCHA, Jan - NOVOTNÝ, Jan - KOMOROVSKÝ, Stanislav - STRAKA, Michal** - KAUPP, Martin** - MAREK, Radek**. Relativistic heavy-neighbor-atom effects on NMR shifts: Concepts and trends across the periodic table. In Chemical Reviews, 2020, vol. 120, no. 15, p. 7065-7103. (2019: 52.758 - IF, Q1 - JCR, 20.847 - SJR, Q1 – SJR) https://doi.org/10.1021/acs.chemrev.9b00785

Korenko Michal, Netriová Zuzana, Šimko František: The award of the presidency of the Slovak Academy of Sciences for the top publication of the Slovak Academy of Sciences, in the category „Publications in scientific journals registered in the Nature Index database“. Ing. RAKHMATULLIN, A** - ŠIMKO, F.** - VERON, E. - ALLIX, M. - MARTINEAU-CORCOS, C. - FITCH, A. - FAYON, F. - SHAKHOVOY, R.A. - OKHOTNIKOV, K. - SAROU-KANIAN, V. - KORENKO, M. - NETRIOVÁ, Z. - POLOVOV, I.B. - BESSADA, C. X-ray diffraction, NMR studies, and DFT calculations of the room and high temperature structures of rubidium cryolite, Rb3AlF6. In Inorganic Chemistry, 2020, vol. 59, no. 9, p. 6308-6318. (2019: 4.825 - IF, Q1 - JCR, 1.349 - SJR, Q1 - SJR, CCC). https://doi.org/10.1021/acs.inorgchem.0c00415

Madejová Jana: Gold medal of the SAS (28. september 2021), granted by the Presidency of the Slovak Academy of Sciences

2.4. Research grants and other funding resources

(List type of project, title, grant number, duration, total funding and funding for the institute, responsible person in the institute and his/her status in the project, e.g. coordinator “C”, work package leader “W”, investigator “I”. Add information on the projects which are interdisciplinary, and also on the joint projects with several participating SAS institutes)

- **International projects**

2.4.1. List of major projects of Framework Programmes of the EU (which pilar), NATO, COST, etc. Add information on your activities in international networks

EU programmes

NOTE – funding is given only for the years within evaluated period 2016-2021, even if the duration of the projects exceeds the years 2016-2021

Sodium-Ion and sodium Metal Batteries for efficient and sustainable next-generation energy storage
Program and grant number: Horizon 2020 963542
Acronym: SIMBA
Duration: 1.1.2021 – 31.12.2024
Funding for the institute: 37 038 € (planned funding for whole duration 138 938 €)
Project coordinator: Technische Universität Darmstadt, Germany
Responsible person from IIC: doc. Ing. Lenčéš Zoltán, PhD. (status – I)
Partners: Germany (Karlsruhe Institute of Technology, Fraunhofer-Institut für Solare Energiesysteme), France (Commissariat à l'énergie atomique et aux énergies alternatives, Saft Groupe S.A., TES-Recupyl SAS), Great Britain (University of Birmingham, University of Warwick, Johnson Matthey PLC), Netherland (Uniresearch BV), Norway (Institute for Energy Technology, Elkem ASA), Sweden (Uppsala University, Altris AB), Ukraine (Yunasko-Ukraine LLC)
The project is interdisciplinar and combines **material engineering, physics, chemistry**. The role of the Institute is to develop novel porous ceramic anode for Na batteries.

New Generation Ultra-High Temperature Ceramic Matrix Composites for Aerospace Industry
Program: Horizon 2020, Marie Sklodowska-Curie (MSCA) 798651
Acronym: CeramCom
Duration: 1.6.2018 – 31.5.2020
Funding for the institute: 145 661 €
Project coordinator: Ing. Tatarko Peter, PhD.
The project had a strong interdisciplinary nature as progress depended upon the combination of **materials science** and **materials chemistry** to develop a series of novel ultrra-high temperature ceramics for aerospace industry (**engineering**). New knowledge in **solid-state physics** on the effect of cation size of RE^{3+} on the ultra-high temperature properties of materials was generated. The main

role of the institute was focused on the synthesis and preparation of new RE-modified ultra-high temperature ceramic matrix composites.

Pushing the envelope of nuclear magnetic resonance spectroscopy for paramagnetic systems. A combined experimental and theoretical approach (pNMR)
Program: FP7 PITN-GA-2012-317127 Marie Curie Action: Initial Training Networks
Acronym: pNMR
Duration: 1.1.2013 – 31.12.2016
Funding for the institute: 40 605 €, 6 393 € from national sources
Project coordinator: Centre Europeen de RMN a Tres Hauts Champs, France
Responsible person from IIC SAS: Dr. Malkin Vladimír, DrSc.
Partners: Germany (TU Berlin, Bruker Biospin GMBH), Finland: OULUN Yliopisto, France (CNRS Lyon), Great Britain (University of Cambridge), Switzerland (ETH Zurich), Italy (Consorzio Interuniversitario Risonanze Magnetiche di Metallo Proteine, Giotto Biotech) Netherlands (Universiteit Leiden), Sweden (Stockholms Universitet)
The goal of the project was to organize a network combining 9 academic research groups and 4 collaborating industrial companies to train the next generation of PhD students and post-doctoral researchers, in developing and applying novel experimental and theoretical methods in the NMR spectroscopy of systems containing paramagnetic metals. The assembled team, with researchers distributed throughout the EU, will investigate a variety of important problems in chemistry and biology including catalysts, battery materials, metalloproteins and large protein-protein assemblies. In this highly multidiscplinary project the role of the instiute was the delopment and implementation of the state-of-art methods for calcularions of paramgnetic NMR parameters.

Building-up Centre of Excellence for advanced materials application — CEMEA
Program: 664337 - H2020-WIDESPREAD-2014-1
Duration: 1.6.2015 – 30.6.2016
Total funding/funding for the institute: 29 444 664 €
Project coordinator: Slovak Academy of Sciences
Responsible person from IIC SAS: doc. Ing. Boča Miroslav, DrSc. (status – W)
Partners: Finland (Teknologian tutkimuskeskus VTT OyEspo, HELSINGIN YLIOPISTO), Slovakia
Partners from SAS: Institute of Physics, Institute of Electrical Engineering, Polymer Institute, Institute of Materials and Machine Mechanics, Institute of Virology
Joint project of several institutes of Slovak Academy of Sciences
The project is interdisciplinar and combines material engineering, physics, chemistry. The role of the Institute is to develop novel advanced ceramics materials.

COST projects

Our Astro-Chemical History
Program: CMST COST Action CM1401
Duration: 26.11.2014 – 25.11.2018
Funding for the institute: 10 757 €
Project coordinator: Institut de Planétologie at dAstrophisique de Grenoble, France
Responsible person from IIC SAS: prof. RNDr. Noga Jozef, DrSc. (status – I)
Partners: Austria (University of Innsbruck), Czech Republic (Institute of Chemical Technology Prague), Germany (Max-Planck Institute of Extraterrestrial Physics Giessenbachstrae), Denmark (Niels Bohr Institute Copenhagen), Finland (University of Helsinki), Hungary (Etvs Iniversity Budapest), Ireland (National University of Ireland), Italy (University of Perugia), Netherland (Kapteyn Astronomical Institute)
The aim of this Action was to bring together laboratory and theoretical gas phase and surface chemistry as well as large facilities based experiments with the aim of rationalizing the molecular evolution. The role of IIC SAS was focused to calculation of highly accurate potential surfaces to study weak intermolecular interactions in the gas phase.

New generation biomimetic and customized implants for bone engineering
Program: MPNS COST Action MP1301
Duration: 1.2.2014 – 31.10.2017
Funding for the institute: 6 125 €
Project coordinator: Belgium Ceramic Research Centre Mons
Responsible person from IIC SAS: prof. RNDr. Šajgalík Pavol, DrSc. (status – I)
Partners: Austria, Belgium (Université Catholique de Louvain), Canada (Ryerson University), Germany (Institute innovative oral surgery and Medicine, RWTH Aachen University Hospital, Institute for Manufacturing Technologies of Ceramic Components and Composites), Denmark (Danish Technological Institute, Technical University of Denmark), Spain (AzureBio S L, Instituto de Ceramica y Vidrio, Histocell S L,Hospital Clinico San Carlos, Universitat Politècnica de Catalunya Barcelona TECH), Finland (University of Tampere), France (Anthogyr, Biotech International, CIRIMAT-ENSIACET, Service Recherche & développement, Dental University of Lyon, Ecole Nationale Supérieure des Mines de Saint-Etienne, Hôpital Dupuytren, Laboratoire d'ingnierie Osto-Articulaire et Dentaire, PCAS, Polyshape, Université de Lille 2, Université de Limoges, Université de Lyon, Université de Valenciennes), Great Britain (Corinthian Surgical Ltd, Newcastle University, Imperial College of London, Queen Mary University of London, The University of Leeds, University of Nottingham), Switzerland (AO Research Institute Davos), Ireland (Stryker Orthopaedics, University of Limerick), Iceland (University Hospital Reykjavik), Italy (Bionica Tech s r l, ISTEC-CNR, Politecnico di Torino, Research Institute Codivilla-Putti, Rizzoli Orthopaedic Institute, University of Bologna), Lithuania (Lithuanian University of Health Sciences), Latvia (Riga Technical University), Netherland (FT Innovations BV, Radboud University Nijmegen Medical Centre), Norway, Portugal (Fluidinova SA, Medbone-Medical Devices Lda, Universidade de Aveiro, Universidade do Porto), Slovenia (Jozef Stefan Institute), Sweden (Stockholm University, Swerea IVF AB), USA (Missouri University of Science & Technology)
The project is highly interdisciplinar and combines biochemistry, inorganic and organic chemistry, medicine, virology. The role of the institute was to prepare trabecular bone-like porous silicon nitride based materials which can be used as bone implants.

- **National projects, incl. international projects with only national funding**

2.4.2. List of ERA-NET projects funded from SAS budget

Graphene-ceramic composites for tribological application in aqueous environments
Program: ERANET, (M-ERA.NET Transnational Call 2013)
Acronym: GRACE
Duration: 1.9.2014 – 31.8.2017
Total funding/funding for the institute: 13 000 €
Responsible person from IIC SAS: prof. RNDr. Šajgalík Pavol, DrSc. (status – I)
Project coordinator: Fraunhofer-Gesellschaft, Freiburg, Germany
Partners: Freiburg Materials Research Center, University of Freiburg, Germany, Institute of Physics, University of Freiburg, Germany, FCT Hartbearbeitungs GmbH, Germany, Institute for Technical Physics and Materials Science, Hungarian Academy of Sciences, Hungary
The project is interdisciplinary combining materials engineering, tribology, inorganic chemistry and fatique of materials. The role of the institute was to prepare silicon carbide and silicon nitride based composites containing graphene platelets in the range of 1 – 10 wt%.

Multifunctional ceramic/graphene thick coatings for new emerging applications
Program: ERANET (call FLAG–ERA JTC 2017)
Acronym: CERANEA
Duration: 1.1.2018 – 31.12.2020
Total funding/funding for the institute: 31 502 € (EU source)
Project coordinator: Institute for Technical Physics and Materials Science, Centre for Energy Research, Hungarian Academy of Sciences (MTA EK)
Responsible person from IIC SAS: doc. Ing. Lenčéš Zoltán, PhD. (status – I)

Partners: Germany (Fraunhofer IKTS), Hungary,
Partners from SAS institutes: Institute of Materials Research SAS Košice Slovakia
The project is interdisciplinary combining materials engineering, tribology, inorganic chemistry and fatique of materials. The materials were suitable for electric discharge machining. The role of the institute was to prepare silicon carbide based composites containing graphene platelets or graphene oxide in the range of 1 – 15 wt% with controlled electrical conductivity

2.4.3. List of projects of the Slovak Research and Development Agency, APVV

Multilateral SRDA (APVV) projects

Relativistic effects in molecular materials based on gold complexes: catalytic activity, proton transfer, and NMR properties
Program: DS-2016-0009 Funding Multilateral Scientific and Technological Cooperation Projects in the Danube Region
Duration: 1.1.2017 – 31.12.2018
Funding for the institute: 3 449 €
Responsible person from IIC SAS: Dr. Malkin Oľga, DrSc. (status – C)
Partners: Austria Paris-Lodron University of Salzburg, Czech Republic: Masaryk University Brno
The project enabled an efficient collaboration between the application laboratories in Austria and Czech Republic with the methodological and development contribution from the theoretical group in Slovakia. The project combined theoretical and experimental studies of gold clusters related to their catalytic activity. The task of the institute was the development of novel computational tools for the prediction and interpretation of NMR parameters.

Bilateral SRDA (APVV) projects – supporting mobility of researchers

Spin Coupling Advanced Level Perception
Project number: SK-FR-19-0001
Duration: 1.2.2020 / 31.12.2022
Funding for the institute: 0 €
Responsible person from IIC SAS: Dr. Malkin Oľga, DrSc.
Partner: Institute of Molecular Chemistry of the University de Bourgundy, France
The project combined advanced experimental techniques of the French partners and quantum-chemical analysis of spin-spin coupling pathways (provided by the institute) in organic and organo-metallic models related to metal/ligand catalysis processes. The project combined theoretical and experimental chemistry.

Ultra-high temperature carbides for extreme environment applications
Project number: SK-SRB-18-0022
Duration: 1.1.2019 / 31.12.2021
Funding for the institute: 3 976 €
Responsible person from IIC SAS: Ing. Tatarko Peter, PhD.
Partners: Vinča Institute of Nuclear ciences, University of Belgrade, Belgrade, Serbia
The project had an interdisciplinary nature, as the ultimate aim of the project, wchich was the development of new carbides for extreme applications, was reached by the combination of materials science, materials chemistry, and solid-state physics. The main role of the institute lied in the densification of carbides with new, unique compositions, as well as their phase and compositional analysis.

Joining of advanced SiC-based ceramic materials
Project number: SK-CN-2017-0040
Duration: 1.1.2018 / 31.12.2019
Funding for the institute: 6 127 €
Responsible person from IIC SAS: Ing. Tatarko Peter, PhD.

Partner: Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, China
The project was multidisciplinary, since the knowledge in materials science, materials chemistry and solid-state physics was combined to reach the main objective of the project, i.e. the development of new, realiable and user-friendly methods to join SiC-based ceramics for nuclear applications. The main role of the institute was focused on the development of solid-state diffusion bonding of the materials.

New technology in Aluminium production – Physicochemical and electrochemical investigation of promising potassium cryolite molten systems
Project number: SK-CN-2015-0014
Duration: 1.1.2016 / 31.12.2017
Funding for the institute: 5 253 €
Responsible person from IIC SAS: Ing. Kubíková Blanka, PhD.
Partner: Key Laboratory for Ecological Metallurgy of Multimetallic Mineral, Shenyang, China

General Calls – IIC SAS as coordinator

Nanostructured, functionally graded, and bioinspired 3D Ti-based implants
Program: APVV-20-0322
Duration: 1.8.2021 – 30.6.2025
Total funding/funding for the institute: 22 333 € / 14 750 €
Responsible person from IIC SAS: doc. Ing. Hnatko Miroslav, PhD.
Project coordinator: Alexander Dubček University Trenčín

Bionanocomposites based on organic polycations and layered silicates
Program: APVV-19-0487
Duration: 1.7.2020 – 30.6.2024
Total funding/funding for the institute: 73 879 € / 41 100 €
Responsible person from IIC SAS: RNDr. Madejová Jana, DrSc. (status – C)
Partner: Institute of Polymers SAS
Interdisciplinar project – material science/inorganic chemistry/polymer science
Role of IIC team: Preparation of materials based on layered silicates and selected organic polycations

Interaction of fluoride melts of rare earth elements with oxides of critical elements in the context of special applications
Program: APVV-19-0270
Duration: 1.7.2020 – 30.6.2024
Total funding/funding for the institute: 110 000 € / 110 000 €
Responsible person from IIC SAS: doc. Ing. Boča Miroslav, DrSc. (status – C)
Role of IIC team: To study the interaction of molten fluorides of selected elements from the group of critical raw materials (defined by the European Raw Materials Initiative) with their oxides. Such systems are currently in use or are being developed for their use in key industries such as metal production, energy applications or corrosion protection.
Interdisciplinar project – material science/inorganic chemistry

Development of the bioactive silicon nitride by surface modification
Program: APPV-18-0542
Duration: 1.7.2019 – 31.12.2022
Total funding/funding for the institute: 167 425 € / 133 425 €
Responsible person from IIC SAS: Mgr. Tatarková Monika, PhD. (status – C)
Partner: Center for Advanced Materials Application SAS, Bratislava
The project has a strong interdisciplinary nature, as the development of new bioactive silicon nitride depends on the knowledge and expertise in materials science, materials chemistry and biomaterials.

The role of the institute is to transform bioinert ceramics, silicon nitride, into the bioactive materials, by the introduction of selected and appropriate bioactive additives.

Development of refractory pyrochlore phases for high temperature applications of non-oxide ceramics
Program: APVV-17-0328
Duration: 1.8.2018 – 30.6.2022
Total funding/funding for the institute: 215 855 € / 150 555 €
Responsible person from IIC SAS: Ing. Tatarko Peter, PhD. (status – C)
Partner: Institute of Materials Research SAS, Košice
In this project, the expertise of the research team in **materials science** were combined with their knowledge and experiences in **materials chemistry** to develop a series of novel diborides for aerospace industry (**engineering**). The main role of the institute was to design and syntesize new diboride based composites reinforced by rare-earth based additives.

Nanocomposite materials based on organo-phosphonium smectites and polymers
Program: APVV-15-0741
Duration: 1.7.2016 – 31.12.2020
Total funding/funding for the institute: 250 000 € / 150 000 €
Responsible person from IIC SAS: Mgr. Jankovič Ľuboš, PhD. (status – C)
Partner from SAS: Institute of Polymers SAS
Interdisciplinar project – material science/inorganic chemistry/polymer science
Role of IIC team: Preparation of materials based layered silicates modified with non-commericial surface active compounds and systematic study of their properties, expecially comparison of thermal stability after loading of selected surfactants to the interlayer of layered silicates.

Advanced composite coatings for high temperature corrosion protection of metals
Program: APVV-15-0014
Duration: 1.7.2016 – 31.10.2020
Total funding/funding for the institute: 249 924 € / 90 000 €
Responsible person from IIC SAS: prof. Ing. Galusek Dušan, DrSc. (status – C)
Partners: Alexander Dubček University Trenčín,
Partner SAS: Institute of Materials Research SAS
The aim of this project was development of new types of composite anti-corrosion protective layers, based on ceramics prepared by controlled pyrolysis of organosilicon precursors. So, the expertise of the research team in **materials science** were combined with their knowledge and experiences in **materials chemistry**.

Fluoride melts of critical elements for unconventional applications
Program: APVV-15-0479
Duration: 1.7.2016 – 31.8.2020
Total funding/funding for the institute: 250 000 € / 250 000 €
Responsible person from IIC SAS: doc. Ing. Boča Miroslav, DrSc. (status – C)
Role of IIC team: Detailed physico-chemical and thermo-chemical analysis of the systems in molten state; spectral and diffraction analysis of formed phases and study of corrosion resistance of different construction materials (alloys, ceramics and binary compounds) under interaction with studied melts.
Interdisciplinar project – material science/inorganic chemistry

The behaviour of new progressive construction materials in aggressive environment of molten salts
Program: APVV-15-0738
Duration: 1.7.2016 – 31.8.2020
Total funding/funding for the institute: 249 689 € / 150 000 €
Responsible person from IIC SAS: Ing. Šimko František, PhD. (status – C)
Partner SAS: Insitute of Physics SAS

Developing new theoretical tools for prediction and interpretation of EPR and NMR parameters

Program: APVV-15-0726
Duration: 1.7.2016 – 30.6.2020
Total funding/funding for the institute: 174 460 € / 156 460 €
Responsible person from IIC SAS: Dr. Malkin Vladimír, DrSc. (status – C)
Partner: Chemical Institute SAS
The main goal of this interdisciplinary project was to improve the accuracy in calculations and interpretation of EPR and NMR parameters. That work was done by the institute. The new theoretical tools were applied for interpretation of NMR parameters obtained experimentally in Chemical Instituite SAS.

Assessment of secondary raw materials for the preparation of materials used in extreme conditions
Program: APVV-15-0540
Duration: 1.7.2016 – 30.6.2020
Total funding/funding for the institute: 164 274 € / 164 274 €
Responsible person from IIC SAS: doc. Ing. Hnatko Miroslav, PhD. (status – C)

Silicon oxynitride-based photoluminescent ceramic materials
Program: APVV-14-0385
Duration: 1.7.2015 – 30.6.2019
Total funding/funding for the institute: 218 088 € / 123 053 €
Responsible person from IIC SAS: doc. Ing. Lenčéš Zoltán, PhD. (status – C)
Partner: Institute of Electrical Engineering SAS, Institute of Materials Research SAS

General Calls – IIC SAS as partner

Bentonite: Slovak strategic raw material – Innovative assessment of bentonite quality and origin for its efficient use
Program: APVV-20-0175
Funding for the institute: 3 550 €
Duration: 1.7.2021 – 30.6.2025
Project coordinator: Faculty of Natural Sciences Comenius University
Responsible person from IIC SAS: RNDr. Madejová Jana, DrSc.
Partner SAS: The Earth Science Institute SAS
Partner: Slovak University of Technology Bratislava

Carbon-silicon based composite anodes for Li-ion batteries
Program: APPV-19-0461
Duration: 1.7.2020 – 30.6.2024
Funding for the institute: 9 703 €
Project coordinator: CEMEA SAS
Responsible person from IIC SAS: doc. Ing. Lenčéš Zoltán, PhD.
Partners: Institute of Physics SAS, Institute of Polymers SAS, Inst. of Electrical Engineering SAS, Institute of Materials and Machine Mechanics SAS

New high – entropy ceramics for advanced applications
Program: APPV-19-0497
Duration: 1.7.2020 – 30.6.2024
Funding for the institute: 28 300 €
Project coordinator: Institute of Materials Research SAS, Košice
Responsible person from IIC SAS: prof. RNDr. Šajgalík Pavol, DrSc.

Advanced materials with eutectic microstructure for high temperature and functional applications
Program: APVV-19-0010
Duration: 1.7.2020 – 30.6.2024
Total funding/funding for the institute: 27 550 €

Project coordinator: Alexander Dubček University Trenčín
Responsible person from IIC SAS: Ing. Prnová Anna, PhD.
The project deals with preparation of materials with exceptional high temperature mechanical properties, and possibly also intensive luminescnece in a broad range of electromagnetic spectra, and identification of relations between preparation conditions, chemical composition, microstructure (**material chemistry**), and properties of these materials (**material science**).

Polymer surfaces modified with layered nanoparticles and photoactive dyes
Program: APVV-18-0075
Duration: 1.7.2019 – 30.6.2023
Funding for the institute: 45 600 €
Project coordinator: Faculty of Natural Sciences Comenius University
Responsible person from IIC SAS: Ing. Pálková Helena, PhD.
Interdisciplinary basic research on multicomponent materials prepared from layered silicates and dyes on the surface of technical polymers. The surface functionality is achieved by suitably selected dyes with interesting photophysical and photochemical properties. The goal is to obtain surfaces which are attractive in terms of possible applications such as photosensitizing and photo-disinfecting properties, luminescent surfaces, systems capable of intermolecular light energy resonance transfer, etc.

Novel glass and glass-ceramic rare-earth aluminates-based phosphors for energy-savin solid state lighting sources emitting while light (pc-WLEDs)
Program: APVV-17-0049
Duration: 1.8.2018 – 31.7.2022
Project coordinator: Alexander Dubček University Trenčín
Funding for the institute: 39 300 €
Responsible person from IIC SAS: prof. Ing. Galusek Dušan, DrSc.
The project is focused on research and development of novel glass and glass-ceramic rare-earth aluminates-based luminescent materials for white light-emitting diodes (pc-WLED), especially materials with efficient red emission, which could improve CRI index compared to the known commercially produced phosphors. The project combines **material science** and **material testing**.

Ceramic materials for extreme operating conditions
Program: APV-15-0469
Duration: 1.7.2016 – 31.12.2020
Funding for the institute: 88 480 €
Project coordinator: Institute of Materials Research SAS, Košice
Responsible person from IIC SAS: prof. RNDr. Šajgalík Pavol, DrSc.

Prevention and eradication of microbial biofilms in relationship to nanomaterials
Program: APVV-15-0347
Duration: 1.7.2016 – 31.12.2020
Funding for the institute: 88 000 €
Project coordinator: Faculty of Natural Sciences Comenius University
Responsible person from IIC SAS: prof. RNDr. Bujdák Juraj, DrSc.

Perlite genesis and innovative approaches to its exploitation and processing
Program: APVV-0339-12
Duration: 1.10.2013 – 30.9.2017
Total funding/funding for the institute: 17 332 €
Project coordinator: Faculty of Natural Sciences Comenius University
Responsible person from IIC SAS: RNDr. Madejová Jana, DrSc.
Partners: Faculty of Mining, Ecology, Process Control and Geotechnologies of the Technical University of Košice, Geological Institute SAS
Role of IIC SAS team: development of procedure to characterize content of water in raw perlites using infared spectroscopy, application of the thermal analysis in characterization of water bonding in perlites
Interdiciplinar project combining disciplines of inorganic chemistry and geology

Development SiC based conductive ceramics
Program: APVV-0108-12
Duration: 1.10.2013 – 30.9.2017
Funding for the institute: 26 150 €
Project coordinator: Institute of Materials and Machine Mechanics SAS Bratislava
Responsible person from IIC SAS: prof. RNDr. Šajgalík Pavol, DrSc.
Partner: Alexander Dubček University Trenčín

2.4.4. List of projects of the Scientific Grant Agency of the Slovak Academy of Sciences and the Ministry of Education, VEGA (for funding specify only total sum obtained from all VEGA grants in particular year)

Year	2016	2017	2018	2019	2020	2021
Funding (€)	109 362	107 600	111 592	102 712	106 482	117 088

IIC SAS – coordinator of projects

- Electromagnetic shielding properties of functionally graded layered SiC-graphene and SiC-carbon nanotubes composites, VEGA 2/0007/21, 1.1.2021 – 31.12.2024, 8 403 €, Ing. Hanzel Ondrej, PhD.
- Ion exchange strengthened aluminosilicate glass/glass-ceramics with additional functionalities, VEGA 2/0028/21, 1.1.2021 – 31.12.2024, 7 409 €, prof. Ing. Galusek Dušan, DrSc.
- Advancing in calculation and interpretation of spectroscopic parameters of heavy element compounds, VEGA 2/0135/21, 1.1.2021 – 31.12.2024, 15 869 €, Dr. Malkin Oľga, DrSc.
- Potential of layered aluminosilicates as excellent guests to accommodate polymeric cations: design of new composite materials, VEGA 2/0166/21, 1.1.2021 – 31.12.2024, 17 853 €, Ing. Pálková Helena, PhD.
- Phase changes of metal oxides in fluoride melts, VEGA 2/0024/20, 1.1.2020 – 31.12.2023, 40 212 €, doc. Ing. Boča Miroslav, DrSc.
- Structure and properties of bioactive glasses doped with ions with potential therapeutic and antibacterial effects, VEGA 2/0164/, 1.1.2020 – 31.12.2023, 1 234 €, doc. Ing. Chromčíková Mária, PhD.
- Development and characterisation of spherical microparticles for preparation of advanced 3D glass and glass-ceramic structures, VEGA 1/0456/20, 1.1.2020 – 31.12.2023, 4 704 €, Ing. Michálková Monika, PhD.
- Insight into the mechanism of interactions of pollutants adsorbed on the surface of aluminosilicate structures, VEGA 2/0021/19, 1.1.2019 – 31.12.2022, 20 964 €, Ing. Scholtzová Eva, CSc.
- Fluoride melts with potential applications in electrochemical aluminum production, VEGA 2/0060/18, 1.1.2018 – 31.12.2021, 41 642 €, Ing. Šimko František, PhD.
- Photoluminescent transparent oxynitride-based ceramics, VEGA 2/0164/18, 1.1.2018 – 31.12.2021, 51 197 €, doc. Ing. Lenčéš Zoltán, PhD.
- Preparation and characterization granuls/microspheres based on silicon nitride for bioapplications, VEGA 2/0152/18, 1.1.2018 – 31.12.2021, 35 904 €, doc. Ing. Hnatko Miroslav, PhD.
- Functionalization of clay minerals using unconventional organic surfactants, VEGA 2/0141/17, 1.1.2017 – 31.12.2020, 84 706 €, RNDr. Madejová Jana, DrSc.
- Transparent polycrystalline ceramics materials with submicrone microstructure and with luminiscent properties, VEGA 2/0026/17, 1.1.2017 – 31.12.2020, 26 3319 €, prof. Ing. Galusek Dušan, DrSc.
- Development of advanced tools for calculation and interpretation of NMR and EPR spectra of heavy element compounds, VEGA 2/0116/17, 1.1.2017 – 31.12.2020, 54 442 €, Dr. Malkin Oľga, DrSc.
- Photoactive hybrid materials, VEGA 2/0156/17, 1.1.2017 – 31.12.2019, 17 887 €, Mgr. Czímerová Adriana, PhD.

- Molten fluoride systems with higher functionality, VEGA 2/0114/16, 1.1.2016 – 31.12.2019, 81 969 €, doc. Ing. Boča Miroslav, DrSc.
- Structure abd properties of oxide glasses – thermodynamic models, entalpic and structural relaxation, VEGA 2/0088/16, 1.1.2016 – 31.12.2019, 7 095 €, doc. Ing. Chromčíková Mária, PhD.
- New rare-earth aluminate-based inorganic phosphors for applications in white light emitting LEDs, VEGA 1/0631/14, 1.1.2014 – 31.12.2017, 8 060 €, Ing. Klement Róbert, PhD.
- Hybrid materials based on layered silicates with cyanine and porphyrine dyes VEGA 2/0107/13, 2013 - 2017, 11 374 €, Mgr. Czímerová Adriana, PhD.
- Improvement of functional properties of ceramic materials with the addition of carbon nano-tubes and graphene, VEGA 2/0065/14, 2014-2017, 14 361 €, doc. Ing. Hnatko Miroslav, PhD
- Ternary silicon nitride and oxynitride-based phosphors, VEGA 2/0112/14, 2014-2017, 22 588 €, doc. Ing. Lenčéš Zoltán, PhD
- Low melting electrolytes and wetted cathodes with potential for electrolytic aluminium production, VEGA 2/0116/14, 2014-2017, 22 433 €, Ing. Šimko František, PhD.
- Preparation and properties of novel organoclays for polymer and environmental applications VEGA 2/0132/13, 2013 - 2016, 22 052 €, RNDr. Madejová Jana, DrSc.
- ReSpect - a practical and efficient computational tool to study heavy element compounds VEGA 2/0148/13, 2013 – 2016, 12 488 €, Dr. Malkin Oľga, DrSc.

IIC SAS - partner

- Corrosion and weathering of tablewareglass, VEGA 1/0064/18, 1.1.2018 – 31.12.2021, 11 069 €, doc. Ing. Chromčíková Mária, PhD.
- Long persistent phosphors on the base of stoichiometric aluminates and silicates for optical and biomedical applications, VEGA 1/0527/18, 1.1.2018 – 31.12.2021, 16 631 €, prof. Ing. Galusek Dušan, DrSc.
- Ceramic coatings with glass fillers for high temperature corrosion protection of metals, VEGA 2/0058/14, 01/2014-12/2016, 5 623 €, prof. Ing. Dušan Galusek, PhD.

2.4.5. List of projects supported by EU Structural Funds

CEMEA – Building a centre for advanced material application SAS, EU Structural Funds, Research and Inovations, NFP313020T081, 1.7.2019 – 30.6.2023, 108 069 €, doc. Ing. Hnatko Miroslav, PhD.

CEDITECH2 - Support of R&D activities of the Centre for quality testing and diagnostics of materials, ITMS project code: 313011W442, duration 2019-2023, 136 224 €, prof. Ing. Dušan Galusek, DrSc.

2.4.6. List of other projects funded from national resources

International - Joint Research Projects (JRP)

Development of functionally graded silicon nitride with improved bioactivity
Program: JRP SAV – TUBITAK 546676
Duration: 1.1.2021 – 31.12.2023
Total funding/funding for the institute: 25 000 €
Responsible person from IIC SAS: doc. Ing. Hnatko Miroslav, PhD.
Partners: TUBITAK Marmara Research Center, Materials Institute, Turkey

Scaffolds and biocomposites for tissue regeneration
Program: SAS-MOST JRP 2018/02
Duration: 1.1.2019 – 31.12.2021
Total funding/funding for the institute: 74 988 €
Responsible person from IIC SAS: prof. Ing. Galusek Dušan, DrSc.
Partners: National Taiwan University, National Taiwan University of Science and Technology

Transparent oxide ceramics with additional optical functionalities
Program: SAS - MOST JRP 2015/06
Duration: 1.1.2016 – 31.12.2018
Total funding/funding for the institute: 74 994 €
Responsible person from IIC SAS: prof. Ing. Galusek Dušan, DrSc.
Partner: NTU Materials Science and Engineering Taipei Taiwan

Development of ceramics composites materials for bio-applications.
Program: SAS - TUBITAK JRP 2013/02
Duration: 1.9.2013 - 31.12.2016
Total funding/funding for the institute: 20 833 €
Responsible person from IIC SAS: prof. RNDr. Šajgalík Pavol, DrSc.
Partner: TUBITAK Marmara Research Center, Materials Institute, Turkey

Atomic Design of Carbon-Based Materials for New Normal Society
Program: V4-Japan Joint Research Program
Acronym: AtomDeC
Duration: 1.11.2021 – 30.10.2024
Funding for the institute: 4 167 €
Project coordinator: Japan: Advanced Institute for Materials Research (AIMR) Tohoku University Sendai
Responsible person from IIC SAS: Ing. Scholtzová Eva, CSc.
Partners: Institute of Fundamental Technological Research; Polish Academy of Science (secondary PI) Warsaw; Poland
Canada: Department of Chemistry, The University of British Columbia, Czech Republic: VŠB-Technical University of Ostrava, Hungary: Faculty of Science and Informatics University of Szeged

Development of new ultra-high temperature ceramic matrix composites with improved oxidatio/ablation properties for aerospace industry
Project number: MVTS 41090027
Duration: 1.11.2017 / 31.10.2020
Funding for the institute: 72 000 €
Responsible person from IIC SAS: Ing. Tatarko Peter, PhD.
- Seal of excellence supporting EU Marie Curie project

Program Mobility
Reaction bonding of advanced SiC-based ceramics
Project number: SAV-AVČR-21-04
Duration: 1.1.2021 - 31.12.2022
Funding for the institute: 1 000 €
Responsible person from IIC SAS: Ing. Tatarko Peter, PhD.
Partner: Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic

MAD – bilateral project based on agreements between academic institutions

Development of new advanced ceramic composites for aerospace industry, MAD 2/0116/17, duration 1.1.2018 - 31.12.2021, responsible person: P. Tatarko, partner: Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic

Development and characterization of a novel glass/ceramic coating systems for high temperatue applications, Program: DAAD, Duration: 1.1.2018 – 31.12.2019, Funding for the institute: 0, Project leader: Universität Bayreuth, Germany, Applicant: D. Galusek, partner

Immobilization of metal nanoparticles on organo-modified layered silicates, MAD 12/2016, responsible person: H. Pálková, partner: Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow, Poland

Other projects

Heat Capacities of fluorozirconate compounds, SFERA3; SURPF2001310039, 1.1.2021 / 31.12.2021, responsible person: Miroslav Boča, partner: ENEA - Casaccia Research Center Italy

DoktoGrant

Corrosion of Superalloys in Energy Application, APP0156, 1.1. – 31.12.2021, funding 2000 eur, responsible person: Ramu Ambati (PhD student)

2.4.7. List of projects funded from private funds

2.4.8. List of projects funded from other competitive funds

2.5. PhD studies and educational activities

2.5.1. List of accredited programmes of doctoral studies, period of validity, source of funding

Institute of Inorganic Chemistry SAS is an external educational institution and has following accredited programmes with three Slovak universities:

1. **Theoretical and computational chemistry** at Faculty of Natural Sciences, Comenius University Bratislava - valid from 24.08. 2021

2. **Inorganic technology and non-metal materials** at Alexander Dubček University of Trenčín – valid from 24.6.2021

3. **Physical chemistry** at Faculty of Natural Sciences, Comenius University Bratislava; – valid from 30.1.2020; at Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava - valid from 4.5.2020

4. **Inorganic chemistry** (Faculty of Natural Sciences, Comenius University Bratislava; Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava) – undeterminate

5. **Inorganic technology and materials** at Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava - undeterminate

6. **Chemical physics** (Faculty of Natural Sciences, Commenius University Bratislava) – undeterminate

Before the legal changes in connection with the new law on higher education, three undeterminate programmes had following guarantors:

RNDr. Peter Komadel, DrSc. – Inorganic chemistry

prof. RNDr. Pavol Šajgalík, DrSc. – Inorganic technology and materials

prof. RNDr. Jozef Noga, DrSc. – Chemical physics

In February 2020, the Scientific board of IIC SAS approved an internal system for evaluating the quality of doctoral studies at the Institute and new guarantors of doctoral study fields are:

doc. Ing. Miroslav Boča, DrSc. – Chemistry (including study programmes: inorganic chemistry, physical chemistry and theoretical and computational chemistry)

Dr. Olga Malkin, DrSc. – Physics (including study programme chemical physics)

doc. Ing. Zoltán Lenčéš, PhD. – Chemical engineering and technolgy (including study programmes: inorganic technology and materials and inorganic technology and non-metal materials).

A budget of Slovak Academy of Sciences is almost the exclusive source of funding of above mentioned programmes. Only one scholarship of PhD student who defeated his doctoral study in chemical physics in the year 2016, was funded by Slovak research and development agency.

2.5.2. Summary table on doctoral studies (number of internal/external PhD students at the end of the year; number of foreign PhD students, number of students who successfully completed their theses during the year, number of PhD students who quit the programme during the year*)*

PhD study	2016			2017			2018			2019			2020			2021		
Number of potential PhD supervisors																		
PhD students	number, end of year	defended thesis	students quitted	number, end of year	defended thesis	students quitted	unumber, end of yea	defended thesis	students quitted	number, end of year	defended thesis	students quitted	number, end of year	defended thesis	students quitted	number, end of year	defended thesis	students quitted
Internal total	6	3	0	6	1	1	8	1	0	9	1	2	12	0	0	13	3	0
from which foreign citizens	1	1	0	1	0	0	2	0	0	5	0	0	8	0	0	11	1	0
External	2	0	0	0	1	1	0	0	0	3	0	0	0	0	0	0	0	0
Other supervised by the research employees of the institute	0	0	0	3	0	0	3	0	0	0	0	0	0	0	0	0	0	0

2.5.3. PhD carrier path – Information on the next career steps of the PhD graduates who received their degree from the institute

In the assessed period, 10 PhD students successfully completed their PhD study. Six of them immediately joined the IIC SAS as researchers: Mgr. P. Boháč, PhD., Ing. M. Kontrík, PhD., Ing. M. Slaný, PhD., Ing. M. Barlog, PhD., D. Moreno Rodriguez, PhD. and Ing. M. Hičák, PhD. The rest were employed in either private (Mgr. L. Petra, PhD., Ing. M. Šimurda, PhD.), governmental (Mgr. M. Vetrecín., PhD) or research companies (P. J. Cherry, PhD.). In all of these cases the obtained PhD degree was a great advantage in their career because they immediately attained leadership or development positions. These graduates established contacts with the employer during their studies and some of them had already started part-time work before their thesis defence or had changed the form of the study to an external one.

List of PhD students:

1. Mgr. Peter Boháč, PhD. – the defence in 08/2016
2. Ing. Martin Kontrík, PhD. – the defence in 08/2016
3. Ing. Michal Slaný, PhD. – the defence in 08/2019
4. Ing. Martin Barlog, PhD. - the defence in 08/2021
5. Ing. Michal Hičák, PhD. – the defence in 08/2021
6. Daniel Moreno Rodriguez, PhD. - the defence in 08/2021
7. Peter John Cherry, PhD. – the defence in 11/2016
8. Mgr. Lukáš Petra, PhD. – the defence in 08/2017
9. Ing. Michal Šimurda, PhD. – the defence in 08/2017
10. Mgr. Michal Vetrecín, PhD. – the defence in 08/2018

The career paths of our colleagues who finished PhDs in previous years can be found on the website of IIC SAS (http://www.uach.sav.sk/about/success-story/) in „Success stories“; entries on this page have been created and supplemented during the period 2016-2021. „Success stories“ present

stories and recommendations of our colleagues or former colleagues about the impact of appointment at IIC SAS on their professional carrier.

2.5.4. Summary table on educational activities

Teaching	2016	2017	2018	2019	2020	2021
Lectures (hours/year)*	17	72	63	91	73	115
Practicum courses (hours/year)*	141	237	231	140	42	52
Supervised diploma and bachelor thesis (in total)	0	2	4	3	3	0
Members in PhD committees (in total)	5	10	7	7	4	6
Members in DrSc. committees (in total)	4	1	1	1	0	2
Members in university/faculty councils (in total)	15	16	16	18	16	16
Members in habilitation/inauguration committees (in total)	3	1	3	2	2	1

2.5.5. List of published university textbooks

2.5.6. Number of published academic course books

2.5.7. List of joint research laboratories/facilities with universities

Joint laboratories:

1. Joint research laboratory on advanced ceramic materials with Northwestern Polytechnical University, Xi-An, China
2. Joint Laboratory of Glass of the Institute of Inorganic Chemistry, Slovak Academy of Sciences with the Faculty of Chemical and Food Technology, Slovak University of Technology and Alexander Dubček University of Trenčín

IIC SAS has two types of **joint facilities with universitites** and **research organizations** obtained within common projects:

- Owned by IIC SAS and shared for other institutions – e.g., XRD spectrometer Panalytical Empyrean, XRF spectrometer ARL Advant'X, thermal analyser STA Jupiter F3, SEM JEOL, AAS spectrometer Varian, ICP OES Varian, UV-VIS-NIR Cary 5000, Fluorescence spectrometer Fluorolog-3, FTIR spectrometer Nicolet 6700, impedance spectrometer Wayne Kerr, gas pycnometer Quantachrome Ultrapyc1200e, FREE ZONE freeze dry system PLUS 2.5 l Cascade, elemental analyzer Horiba EMIA and EMGA, zetasizer Nano ZS 3601 and Brookhaven 90Plus, Renishaw in VIA Raman Microscope, cold, hot and hot isostatic presses, special furnaces for preparation of glass and for physico-chemical properties of molten salts
- Owned by other institutions and shared for IIC SAS – e.g., HRTEM Titan Themis, automatic press KPG 400, cold isostatic press CIP 400-300*750Y, continuous graphite furnace FCW, lapping machine DSG720, Autolab modules – Metrohm, nanointendenr TI-750, Compact XPS/ESCA system, excimer laser Excistar XS, Cone Calorimeter FTT 0005, corrosion chamber SKB-400 A-TR, POWER PULSE pe861DA-50-27-60-S/GD, color and glossmeter SPECTRO-GUIDE 45/0 GLOSS and many others.

2.5.8. Supplementary information and/or comments on doctoral studies and educational activities – focused on what changes have occurred since the last evaluation in 2016

IIC SAS has signed a new framework cooperation agreement regarding doctoral studies with a third university – Alexander Dubček University of Trenčín – and expanded existing framework cooperation agreements with further PhD study programmes – Physical Chemistry (at both Slovak Technical University and Comenius University) and Theoretical and Computational Chemistry at Comenius University.

The number of PhD students is strongly affected by the number of available fellowships from the Presidium of SAS (3), but also by the interest of university students in continuing their studies at the PhD level. Since 2017 IIC SAS has taken the initiative in attracting new PhD students. Besides advertising free PhD positions on the webpage of the Institute and the academic information system of the universities (AIS), PhD topics are promoted on international portals such as Researchgate and Euraxess. As a result of these actions, IIC SAS has an average of 3 new doctoral students per year. Therefore the majority of PhD. students are from abroad. Our PhD topics in 2016-2021 attracted the attention of students coming not only from Slovakia but also from Spain, Greece, Germany, Turkey, Russia, India, Iran, Pakistan and Ecuador (and students from many other countries participated in the interviews for PhD positions).

The structure of the educational activities has changed significantly. The number of hours of laboratory exercises, led by our internal doctoral students, has decreased dramatically. By contrast, the number of hours of lectures given by our scientific staff has increased.

The Institute has persisted in its effort to encourage PhD students to visit cooperating foreign institutions with the aim of gaining experience and skills in the laboratory, learning new methods, etc. The research visits in the period under assessment were:

- M. Barlog: International Center for Materials Nanoarchitectonics (WPI-MANA) at the National Institute for Materials Science (NIMS), Tsukuba, Japan, 14. 07 – 15. 10. 2019, fellowship for PhD. students within NIMS Internship Program.
- M. Kontrík: CEMHTI-CNRS (Conditions Extrêmes et Matériaux: Haute Température et Irradiation), Orléans, France, within the National Scholarship Programme of the Slovak Republic, Slovak Academic Information Agency - SAIA, 10/2015 - 03/2016
- P. Cherry: Magnetic Resonance Center and Department of Chemistry, University of Florence, Italy (13. 3. 2016 – 26. 6. 2016), within project FP7 pNMR, in which the Institute participated.

2.6. Societal impact

2.6.1. The most important case studies of the research with direct societal impact, max. 4 for institute with up to 50 average FTE researchers per year, 8 for institutes with 50 – 100 average FTE researchers per year and so on. Structure: Summary of the impact; Underpinning research; References to the research; Details of the impact; Sources to corroborate the impact. One page per one case study

1. <u>Fundamental understanding of relativistic effects on NMR shifts</u>

Summary of the impact

NMR spectroscopy is one of the basic analytical techniques used in modern chemistry and biochemistry, including those branches oriented toward the improvement of quality of life. Relativistic effects caused by the presence of an atom of a heavy element in a compound can appreciably, even drastically, alter the NMR shifts of the nearby nuclei. A fundamental understanding of such relativistic

effects on NMR shifts, which our research has provided, is important in many branches of chemical and physical science. This understanding is expected to greatly assist experimental chemists and NMR spectroscopists in estimating the ranges of the NMR shifts for unknown compounds, in the identification of intermediates in catalysis or other processes, in analyzing conformational aspects or intermolecular interactions, and in the prediction of trends in series of compounds throughout the Periodic Table. In addition, this newly-obtained fundamental knowledge will contribute to the education of chemistry students.

Underpinning research

The study of spin-orbit relativistic effects on NMR chemical shifts first of all required the development of software which allows one to accurately calculate NMR parameters for systems containing heavy elements, that is, with inclusion of both relativistic effects and the effects of electron correlation. The implementation of theoretical methods must be computationally efficient in order to treat many-electron systems. The software must also provide interpretation tools for the analysis of the obtained results, such as visualization of different properties (*e.g.* for the NMR shielding see Appendix of ref [**1**]) and the decomposition of the calculated values into chemically-meaningful contributions. In addition, the code must allow a user to assess different relativistic effects. All of these required features have been implemented into the in-house ReSpect program [**2**, **3**]. The spin-orbit effects were studied in works [**4**, **5**, **6**], with the concluding article published in one of the most highly regarded and highest-ranked journals to cover the general topic of chemistry.

References to underpinning research

[1] J. Phys. Chem. A **124**, 5157–5169 (2020), DOI: 10.1021/acs.jpca.0c02807
[2] http://www.respectprogram.org/index.html
[3] J. Chem. Phys. **152**, 184101 (2020), DOI: 10.1063/5.0005094
[4] J. Chem. Theory Comput. **13**, 3586–3601 (2017), DOI: 10.1021/acs.jctc.7b00444
[5] J. Chem. Theory Comput. **14**, 3025–3039 (2018), DOI: 10.1021/acs.jctc.8b00144
[6] Chem. Rev. **120**, 7065–7103 (2020). DOI: 10.1021/acs.chemrev.9b00785

Details of the impact

The introduced principles of the spin-orbit effects on NMR shifts of light elements have a general validity across the periodic table. The decades-old question of why compounds with occupied frontier π molecular orbitals cause a shielding effect, while the frontier σ orbitals cause deshielding, is answered. The spin-orbit effects on NMR chemical shifts become easily understandable for a wide chemical audience.

Sources to corroborate the impact

The concluding article [**3**] was published in a journal with an impact factor of 54.564 according to the Journal Citation Reports for 2020. The article, published less than two years ago, has already been cited 42 times and the number of online views of the article exceeds 7870 [https://pubs.acs.org/doi/10.1021/acs.chemrev.9b00785].

The Altmetric Attention Score is a quantitative measure of the attention that a research article has received online. According to Altmetric, reference [**3**] is in the top 10% of all research outputs ever tracked by Altmetric [https://acs.altmetric.com/details/84569446#score].

2. A new industrial electrowinning processes

Summary of the impact

With the estimated increase of the population of our planet by another 2 billion by 2050, the mass production of metals is certain to grow. For a simple comparison, the population increase on our planet of nearly 2 thousand million over the last 40 years has resulted in two times higher production of Fe and Cu and three times higher production of Al. Electrolytic processing is used commercially to recover metals like Al and Mg and refine primary metals like Cu, Ni, and Zn. There are also new and thrilling options for utilizing electrometallurgy in the production of Si, Sc, Ta, Nb and rare earth elements like Nd, Gd, Sm, *etc*. The success of Al production by electrolysis then enabled other metals to become produced by electrolysis, and the prospect of cost-effective C-free electricity offers a completely unique opportunity for a new approach to electrometallurgy. This research in the field of high-temperature molten salts chemistry and electrochemistry is having a direct impact on the industrial performance of existing technologies.

Underpinning research

In the field of metal extraction, our approach to enhancing metal recovery and sustainability consists in operating the separation directly at the reduction step using electricity. In this context, we are currently investigating the development of a new electrochemical route for production of metals in extreme environments. The principle of this process is to extract the elements individually or in the form of alloys in the molten state in an electrolysis cell with molten salt electrolytes, in order to replace the existing capital-intensive and environmentally-harmful operations. The goal of this work is to offer a set of physicochemical data on the new molten salt electrolytes so that the data can be used to further advance physical, chemical, and economical assessments of the new industrial electrowinning processes. The academic outcomes of the work are described in the papers published jointly with our partners from academia [1-9] as well as in the several reports for our industrial partners over the period 2016-2021 [10-11]. Our industrial partners are RIO TINTO, HYDRO, and ALCOA. Each of these partners is a major player in the global aluminium industry.
With respect to corroboration, we quote below from a correspondence with Nancy J. Holt, who leads the Steering Committee at HYDRO related to our project, and Marian Kucharík (HYDRO). The project for our industrial partners (RIO TINTO and HYDRO) was related to the development of the method and measurement of the kinetics of the dissolution of alumina in industrial cryolite electrolytes. Nancy J. Holt is well placed to corroborate the impact and the importance of our outcomes for both industrial partners. She said: “SINTEF also have high regards for this institute, another indication that there must be some capabilities worth supporting. And the fact stands: they did manage to get a method up and running on how to measure alumina quality differences with respect to dissolution rate. Others have not been as successful.”
Note: The term “institute” in this correspondence means IIC SAS. SINTEF is a Norwegian applied research and innovation company - one of the largest research organisations in Europe.

References to the research

[1] Šimko F., et al., Inorg. Chem. **57**(21), 2018, 13702; Doi: 10.1021/acs.inorgchem.8b02275.
[2] Bučko T. and Šimko F., J. Chem. Phys. **148**(6), 2018, 64501; Doi: 10.1063/1.5017106.
[3] Šimko F., et al., J. Chem. Eng. Data **65**(5), 2020, 2642; Doi: 10.1021/acs.jced.0c00023.
[4] Kubíková B., et al., J. Chem. Eng. Data, 63(8), 2018, 3047; Doi: 10.1021/acs.jced.8b00157.
[5] Leonard N., et al., Chem. Eng. Sci., **148**, 2016, 155; Doi: 10.1016/j.ces.2016.03.030.
[6] Korenko M., et al., Energy, **135**(15), 2017, 182; Doi: 10.1016/j.energy.2017.06.044.
[7] Šimko F., et al., J. Mol. Liq., **328**, 2021, 115453; Doi: 10.1016/j.molliq.2021.115453.
[8] Šimurda M., *et* al., *New J. Chem*., **42**(6), 2018, 4612; Doi: 10.1039/C7NJ05156E.
[9] Kubíková B., *et* al., J. Chem. Eng. Data **61**(4), 2016, 1395; Doi: 10.1021/acs.jced.5b00536.
[10] Research reports drawn up as part of the contract between the ICC SAS and RIO TINTO and HYDRO (2017-2021) related to the method development and electrochemical and visual measurement of the kinetics of the dissolution of different industrial aluminas in industrial cryolite electrolyte.
[11] A research report drawn up as part of the contract between the ICC SAS for the ELYSIS joint venture (RIO TINTO, ALCOA and APPLE, 2021) related to the measurement of the ionic and electronic conductivity of the acid cryolite electrolytes for green CO2-free production of aluminium.

3. Microspheres for different applications

Summary of the impact

One of the key pieces of equipment in the VILA Department is a house-built apparatus for flame synthesis of materials. This allows the preparation of spherically-shaped glass particles with a required size range and distribution. The adjustable temperature of the torch over the range from 1400 – 2200 °C with rapid cooling offers the possibility to prepare glasses with a wide range of chemical compositions, including glasses with poor glass forming ability and rapid crystallization kinetics. This way, materials in an amorphous state can be produced in a desired shape for various applications. Microspheres of the glassy system of yttrium aluminium garnet (YAG), prepared by flame synthesis, were for the first time densified at temperatures below 900 °C. Development in the field of bioactive glasses in the system 45S5 led to the fabrication of microporous bioactive glass by using an alkali-activated precursor followed by the flame spheroidization process. Also, the use of flame synthesis allows the preparation of amorphous åkermanite glass microspheres from the glass-ceramic powder, which cannot be prepared by traditional glass melting process. Such materials can be utilized in various applications, from lasers to medical treatment. Interesting results were obtained in the field of white-light-emitting LEDs. The Y_2O_3-Al_2O_3 system, doped with Eu^{2+}/Eu^{3+} ions, provides very promising results. The use of only one rare earth element (RE) ion at a relatively low concentration in the matrix is an undeniable advantage, in contrast to known phosphors where the presence of 2-3 different RE ions in one or more phases is necessary for white light emission. Transparent magnesium-alumina spinel was prepared by low temperature sintering, revealing the role of optically inactive defects in the preparation. New preparation methods and sintering additives enable sintering at lower temperatures to ensure transparency.

Underpinning research

Mastering the fabrication of glass microspheres requires knowledge provided by basic research on the thermodynamics and crystallization kinetics of various types of glasses. Proper adjustment of flame synthesis parameters is vital for obtaining microspheres with the desired features in high yield. For example, the YAG microspheres were produced at the maximum torch temperature of 2200 °C, while a temperature of 1500 °C was sufficient for the preparation of porous bioactive glasses. The research on controlled crystallization was also important for the preparation of white-light-emitting LEDs. Eu^{2+} emits intensely across all wavelengths of visible light, while Eu^{3+} typically emits only red light, so Eu doping in the Y_2O_3-Al_2O_3 matrix results in white light emission; and by tuning the wavelength of the excitation radiation, the fraction of red-light emission in the resulting white light can be increased effectively.

The studies on the preparation of the magnesium-alumina spinel reveal that:

a) SPS at low temperatures reduces the carbon contamination, allowing sintering below 1300°C,
b) structural defects decrease the apparent activation energy of sintering,
c) LiOH promotes the sinterability of spinel and can be used as an alternative to conventional sintering additives,
d) The addition of transition metal fluorides can aid the densification.

References to underpinning research

[1] J. Eur. Ceram. Soc. 37 4271 (2017), Doi: 10.1016/j.jeurceramsoc.2017.05.007
[2] J. Therm. Anal. Calorim. 131 1115–1123 (2018), Doi: 10.1007/s10973-017-6690-9
[3] Mater. Lett. 256, 126625 (2019), Doi: 10.1016/j.matlet.2019.126625
[4] Ceram. Int. 45 23467–23474 (2019), Doi: 10.1016/j.ceramint.2019.08.051
[5] J. Eur. Ceram. Soc. 40 2581-2585 (2020), Doi: 10.1016/j.jeurceramsoc.2019.11.011
[6] J. Eur. Ceram. Soc. 41 1537–1542 (2021), Doi: 10.1016/j.jeurceramsoc.2020.10.015

Details of the impact

The introduced porous glass microspheres have a great potential in various fields and the effect of alkali activation on the pore formation ability have to be better understood also for other systems, representing an opportunity for a breakthrough in preparation of light weight composites, fillers, or materials for direct use. The development in the sintering process, especially in viscous flow sintering at temperatures around 900 °C in the system Y_2O_3-Al_2O_3, leads to a significant decrease of the

preparation cost of transparent materials, usually fabricated above 1600 °C. The principles of the utilization of a proper starting material (shape, composition and purity) in combination with advanced densification techniques could be applied for a variety of diferent glass and glass-ceramic materials.

4. Understanding mechanisms related to dye adsorption / molecular aggregation in colloids

Summary of the Impact

Although the primary objective of the original papers [1,2] of this project was to elucidate the mechanism of molecular aggregation of dyes in colloidal dispersions of layered silicates [3], the results of the latter study [2] yielded much more insight. It shed more light on the nature of the processes accompanying adsorption of molecules on colloidal particles, and thus may contribute to rewriting our basic ideas about the mechanisms associated with adsorption in general. A critical analysis of other theories has also been reported [4].

Underpinning research

The activation energy barrier of molecular aggregation in solutions is very low and the kinetics extremely fast. On the other hand, similar processes in colloidal systems are very slow, which was something of a mystery [4]. Published research on these processes has so far failed to explain this mystery. We chose colloidal dispersions of rhodamine 123 (R123) adsorbed on layered silicate particles as model systems for examining this topic [1,2]. Due to the complex nature of the processes, it was necessary to record several hundred spectra for each reaction, and the accumulated data matrices were analyzed by special chemometric procedures. Although the adsorption of R123 on silicate particles is essentially an instantaneous process, it is accompanied by at least two independent processes leading to slow molecular aggregation. These two independent processes are theorised to be surface and bulk diffusion. Which process predominates depends on various factors, including the reaction conditions [2].

References to underpinning research

[1] Šimonová T., Bujdák J., Clays Clay Miner. 66 (2018) 114–126, Doi: 10.1346/CCMN.2018.064089
[2] Šimonová T., et al. Phys. Chem. Chem. Phys. 23 (2021) 17177–17185, Doi: 10.1039/d1cp02762j
[3] Bujdák, J. Photochem. Photobiol. C 35 (2018) 108–133 Doi: 10.1016/j.jphotochemrev.2018.03.001
[4] Bujdák J., Appl. Clay Sci. 191 (2020) 105630. Doi: 10.1016/j.clay.2020.105630

Details of the Impact

The main study [2] presents the first clear experimental evidence that rapid adsorption can be followed by slow, complex processes related to the redistribution of adsorbed molecules. The effect of various parameters and conditions on the occurrence of these processes was reported [2]. Although this work involved a system based on layered silicate and organic dye, the knowledge gained from it may be important for the interpretation of interface or heterogeneous processes in general, including catalysis, nanotechnologies, and bioorganic colloids or biological systems.

Sources to corroborate the impact

J. Bujdák was invited to write a review article on the topic in a prestigious journal [4]. T. Šimonová Baranyaiová as a PhD student was given an award at the 11th Conference on Colloid Chemistry (Eger, Hungary) in 2018 for the best poster at the conference. The critical analysis of the mechanism of adsorption [4] has received 29 citations. The main work was published in Phys. Chem. Chem. Phys. [1] and became a part of the themed collection “2021 PCCP HOT Articles”. The paper attracted much attention from the scientific community: the editors from the Journal of Physical Chemistry B have recently invited the authors to write a "Perspectives"-type article on this topic.

2.6.2. List of the most important studies and/or other activities commissioned for the decision-making authorities, the government and NGOs, international and foreign institutes (title, name of institution, contract value, purpose (max 20 words))

Individual studies are not listed here; but such reports (at least one per person per year) are an inseparable part of the duties of the following employees who have served as members of such bodies:

doc. Ing. Miroslav Boča, DrSc.
- Ad hoc commission for the defense of doctoral dissertations in the field of Inorganic Chemistry – president (since 2021)

prof. Ing. Dušan Galusek, DrSc.
- Ad hoc commission for the defense of doctoral dissertations in the field of Inorganic Technology and Materials – president since 2021
- Slovak committee for scientific degrees - vice-president

RNDr. Peter Komadel, DrSc.
- Commission for the defense of doctoral dissertations in the field of Inorganic Chemistry – president (till 2019)

Ing. Michal Korenko, PhD.
- Member of the committee for objections in public procurement (Body of the Slovak Government - Office for Public Procurement) - external member

doc. Ing. Zoltán Lenčéš, PhD.
- Sector-driven innovation - National system of professions (belonging to the Ministry of Labour, Social Affairs and Family of the Slovak Republic)

RNDr. Jana Madejová, DrSc.
- Commission for the defense of doctoral dissertations in the field of Inorganic Chemistry president (2019-2021)
- Member of the Council for Natural Sciences; Slovak Research and Development Agency

prof. RNDr. Jozef Noga, DrSc.
- Member of the Working Group for Chemistry and Chemical Technology of the Accreditation Committee of the Slovak Republic (Accreditation Commission Counselling body of the Government of the Slovak Republic)

prof. RNDr. Pavol Šajgalík, DrSc.
- Research agency of Slovak Republic
- Pandemic Commission of the Ministry of Health of the Slovak Republic member
- President of Council of presidents for research priorities, Ministry of Education, Science, Research and Sport of the Slovak Republic - president
- Committee of Ministry of Education, Science, Research and Sport of the Slovak Republic for Awards of Ministry of Education
- Slovak Innovation and Energy Agency
- Slovak committee for scientific degrees - vice-president
- Ad hoc commission for the defense of doctoral dissertations in the field of Inorganic technology and materials - president (till 2021)
- Government Council for Science, Technology and Innovation
- Committee of Ministry of Education, Science, Research and Sport of the Slovak Republic for Awards of Ministry of Education

2.6.3. List of contracts and research projects with industrial and other commercial partners, incl. revenues (study title, name of institution, contract value, country of partner, purpose (max 20 words))

- Supply Contract - Supply of Services - Contract No. CW2119401, Aluminium Pechiney, 120 000.00 €, FRANCE, Mapping of the key industrially aluminium oxide characteristics for optimal dissolution performance
- Supply Contract - Supply of Goods and/or Services - Contract No. CW2119401, Rio Tinto Aluminium Pechiney, 70 000.00 €, FRANCE, Comparison of the dissolution rate of aluminas in cryolite bath using an electrochemical method
- Supply Contract - Supply of Goods and/or Services - Contract No. CW2142413, Rio Tinto Aluminium Pechiney, 29 700.00 €, FRANCE, The conductivity measurements of industrially cryolite based melts
- Statement of work 002 - contract #CW2142413, Rio Tinto Aluminium Pechiney, 17 500.00 €, FRANCE, Alumina dissolution tests in order to transfer this method in company lab in France
- Statement of work 003 - contract #CW2142413, Rio Tinto Aluminium Pechiney, 22 000.00 €, FRANCE, The evaluation of the dissolution rate of 4 different aluminas provided by the Company
- Statement of work 004 - contract #CW2142413, Rio Tinto Aluminium Pechiney, 46 843.00 €, FRANCE, Refurbishment of the furnace for the alumina dissolution experiments
- Cooperation agreement in the research and development, GLASS SERVICE, j.s.c., based on the order, CZECH REPUBLIC, Measurement of temperature dependence of electric conductivity of glass forming melts
- Cooperation agreement, GLASS SERVICE, j.s.c., based on the order, Czech Republic, Measurement of temperature dependence of electric conductivity of glass forming melts
- Research and development of advanced refractory materials based on Al-Si-O-C-N a Zr-O-C-N, RHI AG Leoben, 3 000.00 €, AUSTRIA, Synthesis and characterization of oxinitrides in ordinary ceramic refractories
- Cooperation agreement in the research and development, CONFAL, j.s.c., according to the price list of services, SLOVAKIA, Analysis of waste materials from industrial aluminium electrolysis Project for industrial partner CONFAL, inc. Slovenská Lupča, Slovakia
- Cooperation agreement No. 201705001, CEIT, j.s.c., according to the price list of services, SLOVAKIA, Analysis of optical homogeneity of YAG single crystals. Development of transparent / luminescent polycrystalline ceramic materials that can successfully replace glass and single crystals in the production of rigid lasers, scintillators, or electro-optical devices.
- Cooperation agreement in the research and development, RONA, j.s.c., according to the price list of services, SLOVAKIA, Analysis of defects (stones, cords) in glass products

2.6.4.1 List of intangible fixed assets (internally registered IP (confidential know-how), patent applications, patents granted, trademarks registered) denoting background IPR

2.6.4.2 List of licences sold abroad and in Slovakia, incl. revenues (background IPR identification, name of institution, contract value, country of partner, purpose (max 20 words))

2.6.5. Summary of relevant activities, max. 300 words (describe the pipeline of valorization in terms of Number of disclosure, Number of registered IP internally, number of CCR/LIC contracts and their respective summary values, the support you are receiving in specific points internally at the institute, at SAS, externally – also the limitations and drawbacks.

2.7. Popularisation of Science (outreach activities)

2.7.1. List of the most important popularisation activities, max. 20 items

Appearance in television:

1. Miroslav Boča, F. Šimko, M. Korenko, VAT – Science and Technology, RTVS:2, https://www.rtvs.sk/televizia/archiv/14067/256427#445 16.1.2021
2. Zoltán Lenčéš, Show Science and Technology VAT - SAS scientists are developing new sodium-based batteries, RTVS:2 23.1.2021
3. Miroslav Boča, F. Šimko, B. Kubíková, V. Pavlík, The Spectrum of Science - Modern use of fluoride melts, RTVS: 2 24.11.2018
4. Peter Tatarko, RTVS News – an interview, RTVS 18.2.2018
5. Peter Tatarko, VAT – Science and Technology RTVS 31.3.2018
6. Miroslav Boča, F. Šimko, B. Kubíková, V. Pavlík TV The Spectrum of Science – Modern use of fluoride melts RTVS: STV2 22.10.2016
7. Peter Boháč, RTVS News – interview to Researchers Night event, RTVS 30.9.2016

Appearance in radio broadcasting, interview in podcasts released on internet, videos

8. Stanislav Komorovský, RO Scientific podcast SAS The world of quantum mechanics and the theory of relativity, 8.1.2021 https://www.youtube.com/watch?v=wtzv2IGuamc
9. Miroslav Boča, Michal Korenko, František Šimko, Department of Molten Systems IIC SAS https://www.youtube.com/watch?v=c_EuP1ZyTLE 2.11.2020
10. Peter Boháč, SRo Slovak Radio, Science in two minutes FUN radio https://www.funradio.sk/kategoria/veda-na-2-minuty/ 21.11.2021
11. Juraj Bujdák, SRo Slovak Radio, Night Pyramid – guest in show 30.4.2019

Popularisation articles in printed media or internet media

12. Peter Boháč, No need to fight chemistry. Chemistry, like whole nature, is governed by basic rules that need to be understood Proti chémii netreba bojovať. EDUTECH https://www.eductech.sk/novinky/peter-bohac-proti-chemii-netreba-bojovat-chemia-ako-aj-cela-priroda-sa-riadi-zakladnymi-pravidlami-ktore-treba 16.3.2021
13. Eva Scholtzová, Functional clays and HPC, Hpc Focus: magazine of Computing Centre of Slovak Academy of Sciences (https://vs.sav.sk/magazine/issues/magazine_202101_print.pdf), 1, 2021
14. Miroslav Boča, Michal Korenko, František Šimko, Slovak scientists are studying fluorides for "green" chemistry, Pravda 2.11.2020
15. Miroslav Boča, Elements – known and unknown, ChemZi - journal of Slovak Chemical Society1
16. Peter Tatarko, The scientist has returned to Slovakia after three years in London, and will develop material for supersonic aircraft, Slovakian journal Denník N, 2.3.2018
17. Ľubomír Smrčok, Modern science in our country? magazine Týždeň 24.1.2016

Public popularisation lectures

18. Miroslav Boča, Elements – known and unknown, lecture for students of high schools, Zrkadlový háj, Bratislava 5.12.2018
19. Peter Tatarko, Way to high-temperature materials suitable for space applications vedanadosah.cvtisr.sk 22.3.2018

Excursions and summer schools, scientific events

20. Yearly organised Open Door Day at IIC SAS, with presentation of the results and experiments; involvement of young researchers of IIC SAS in organization of Summer School for young students, participation at European Researchers' Night.

2.7.2. Table of outreach activities according to institute annual reports

Outreach activities	2016	2017	2018	2019	2020	2021	total
Articles in press media/internet popularising results of science, in particular those achieved by the Organization	1	0	7	1	8	2	19
Appearances in telecommunication media popularising results of science, in particular those achieved by the Organization	2	1	4	1	0	3	11
Public popularisation lectures	1	1	4	5	5	0	16

2.8. Background and management. Infrastructure and human resources, incl. support and incentives for young researchers

2.8.1. Summary table of personnel

2.8.1.1. Professional qualification structure (as of 31 December 2021)

	Degree/rank				Research position		
	DrSc./DSc	CSc./PhD.	professor	docent/ assoc. prof.	I.	II.a.	II.b.
Male	6	27	4	5	6	14	11
Female	2	16	0	2	2	8	8

I. – director of research with a degree of doctor of science/DrSc.
II.a – Senior researcher
II.b – PhD holder/Postdoc

2.8.1.2. Age and gender structure of researchers (as of 31 December 2021)

Age structure of researchers	< 31		31-35		36-40		41-45		46-50		51-55		56-60		61-65		> 65	
	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
Male	2.0	2.0	7.0	5.7	5.0	5.0	2.0	2.0	8.0	7.2	1.0	0.6	2.0	1.5	1.0	1.0	5.0	2.5
Female	2.0	2.0	2.0	1.4	1.0	0.8	3.0	2.2	4.0	4.0	2.0	1.6	1.0	1.0	2.0	2.0	0.0	0.0

A – number

B – FTE

2.8.2. Postdoctoral fellowships (list of positions with holder name, starting date, duration. Add brief information about each fellow's career path before and after receiving PhD degree, etc.)

2.8.2.1. MoRePro and SASPRO fellowships

SASPRO support is dedicated for experienced scientists to perform their research at the SAS institutes. SAS Institutes act as host organisations. It consists of two mobility schemes "Reintegration" for Slovakian citizens and "Incoming" for researcher from other countries.

LUMON – Transparent luminescent oxynitrides
Program: SASPRO 1329/03/03, Incoming
Duration: 1.1.2016 – 31.12.2018
Project leader (Host): prof. RNDr. Pavol Šajgalík, DrSc.
Fellowship holder: Dr. Mohamed Radwan (Egypt)
Fellow's career path: as senior researcher Dr. Radwan worked in University of Stockholm (Sweden), after completing his fellowship at IIC SAS he continues in his research work in private company (INFICON Aaland Ab, Finland)

Moving relativistic quantum chemistry out of the shadow: Relativistic paramagnetic NMR
Program: SASPRO 1536/03/02, Reintegration
Duration: 1.10.2016 – 31.12.2018
Project leader (Host): Dr. Malkin Vladimír, DrSc.
Fellowship holder: Dr. S. Komorovský (Slovakia)
Fellow's career path: prior obtaining fellowship applicant received post-doc position in Centre for Theoretical and Computational Chemistry, University of Tromsø - The Arctic University of Norway, after completing his project, presently he is working as senior researcher at the IIC SAS in position of Head of department of theoretical chemistry

HITEMPCORR – High-temperature properties of materials corrosion in molten salts
Program: SASPRO 1119/02/02, Incoming
Duration: 5.11.2015 – 4.11.2018
Project leader (Host): doc. Ing. Boča Miroslav, DrSc.
Fellowship holder: Niketan Sarabhatai Patel (India)
Fellow's career path: prior obtaining fellowship applicant received 6 months post-doc position at Aix-Marseille Universite – CNRS, Marseille (France), after completing his fellowship at IIC SAS he continues in his research work in Saudi Arabia.

2.8.2.2. Stefan Schwarz fellowships

- Mgr. Peter Boháč, PhD. (2020–2022), , Fellow's career path – finished PhD at IIC SAS in 2016, obtained research position at the project at Karlsruhe Institute of Technology, Germany (Sandwich VP project, 01/11/2017 – 06/06/2019).
- Mgr. Silvia Belušáková, PhD. (2019–2021), Fellow's career path: finished PhD in 08/2017, after one year of S. Schwarz fellowship she quited employment at the Institute and continued in the research work in private company Geothermal, j.s.c.

2.8.2.3. Postdoctoral positions from other resources (specify)

Positions funded from Institute´s own sources

- Dr. Oksana Matselko, PhD. (since 03/2021), career path – finished PhD at Faculty of Chemistry, Ivan Franko National University of Lviv, Ukraine in 05/2019
- Ing. Veronika Silliková, PhD. (since 09/2020), career path – finished PhD at Faculty of Natural Sciences, Comenius University, Bratislava, Slovakia in 08/2020

- Mgr. Tímea Šimonová, PhD. (since 09/2019), career path – finished PhD at Faculty of Natural Sciences, Comenius University, Bratislava, Slovakia in 08/2019
- Mgr. Marek Pribus, PhD. (since 09/2019), career path – finished PhD at Faculty of Natural Sciences, Comenius University, Bratislava, Slovakia in 08/2019
- Mgr. Silvia Belušáková, PhD. (09/2017-07/2019), career path – finished PhD at Faculty of Natural Sciences, Comenius University, Bratislava, Slovakia in 08/2017
- Ing. Peter Škorňa, PhD. (since 09/2017) career path – finished PhD at Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Slovakia in 08/2016

SAIA fellowship

Dr. Anna Kityk, PhD. (04/2018-06/2018), career path – finished PhD. at Ukrainian State University of Chemical Technology (Dnipro, Ukraine) in 2013

- 2-months fellowship for international university teachers, researchers and artist from National scholarship program of Slovak republic
- 9-month fellowship occurred between 09/2019-04/2020

2.8.3. Important research infrastructure introduced during the evaluation period with the information about the sources of funding *(max. 2 pages)*

The programming period 2014-2020 for Structural Funds in Slovakia brought significant disappointments. The first problem was the fact that the Bratislava region was specifically excluded from the structural funds, so no infrastructure was eligible for projects. Only partial participation of Bratislava institutes, including our Institute, was allowed, at a maximum level of 15 % of the project budget (for salaries or materials). Enormous administration and unreasonably burdensome requirements presented a significant obstacle to planning and development of the Institute (e.g. the administration required an official public tender for airplane tickets four years in advance for a conference where the venue was not agreed by the organizer, or price offered by the hotel, etc.). In spite of these conditions the Institute spent a lot of time preparing proposals for seven projects (as a partner). In the end, however, the call for projects was cancelled in 2018 due to governmental corruption. The following year, our Institute participated in the preparation of seven different project proposals with different topics and partners (so-called DSV projects). Unfortunately, the call for projects for this round of funding was also cancelled, two years after the initial call, without project evaluation. Thus, we regret to say that, in spite of enormous effort, we were not able to extend our infrastructure.

This means that the majority of the high-tech infrastructure obtained within the framework of EU projects comes from the previous programming period. The instruments are located either in Bratislava or in Trenčín (Department of VILA) and are available not only to IIC but also to researchers from other institutions. It must, however, be emphasised that when in use this infrastructure also requires service and maintenance, entailing additional and somewhat sizeable financial costs.

As a result of the problems outlined above, we focused our attention on at least acquiring or constructing special experimental equipment that is not commercial. Such an approach requires all details of the technical solution to be supplied by us, starting with drawings or diagrams, then proceeding to material supply and construction, and finally putting into operation (including testing and tuning). Thus, we would like to list here some of the infrastructure which the Institute has built or upgraded in the last few years:

1. The furnace that is used for electrochemical monitoring of alumina dissolution in cryolite melts, with the option of direct video observation of the dissolution process (Figure below). This activity was carried out as part of our project with the industrial partners Hydro Aluminum AS (HAL), Oslo, Norway and RioTinto Aluminium Technology Solutions France (ATS), Voreppe, France.

2. During the period 2016-2021 we performed a large upgrade of our local computing capacities. We installed eight servers based on Intel processors and one server based on an AMD processor. In addition, we upgraded the air-conditioning unit and installed a new air-conditioning system that takes advantage of the cold air during winter seasons. For this purpose the following sources of funding were used: SASPRO 1563/03/02, VEGA 2/0116/17, VEGA 2/0135/21, APVV-15-0726, and APVV-19-0516.
3. A unique apparatus was built in-house for surface modification of materials using an oxyacetylene torch. The equipment is capable of testing materials against ablation in an oxidizing environment at temperatures of up to 3000°C. Such a test is widely accepted in the relevant research community as an appropriate primary lab test to investigate the ablation resistance of prospective materials for thermal protection systems of hypersonic vehicles. This helps to select the most promising materials, which are then tested in an arc-heated plasma wind tunnel, simulating the real atmospheric conditions during re-entry of a vehicle. This instrument significantly enhances the international reputation of the Institute and the country in the field of advanced materials for aerospace, as this is the only equipment capable of performing such tests in Slovakia. At the same time, the research team at the institute also found an alternative use of this instrument, namely improving the bioactivity of ceramic materials, which is a unique approach in the field of bioceramics. The importance of the equipment is clearly demonstrated by its multidisciplinary use.
4. IIC SAS is a member of the CEMEA project consortium (for building a centre for advanced material applications for the SAS; EU Structural Funds, Research and Innovations, NFP313020T081, 1.7.2019 – 30.6.2023). In this project, the modernization of the infrastructure was first planned, and then IIC SAS contracted for the supply of several important devices and a number of small devices which will certainly contribute to increasing the quality of scientific outputs at IIC SAS. Of these, the devices we consider most important are: equipment for the preparation of complicated parts by injecting a plastic mixture of metal or ceramic powders and a suitable plasticizer into the mold; a hybrid furnace for hot press / Spark Plasma Sintering; a high-temperature non-graphite vacuum furnace with an electric resistance heating element; and equipment for 3D printing of ceramic components.
5. The institute also invested in the reconstruction of the internal internet network.
6. In spite of the difficult situation described earlier, our Institute reconstructed 4 big laboratories (start 1.2.2019) and 6 offices from our own sources. In addition, the Institute received from the presidency of the SAS some resources for reconstruction of the water supply and sewage system.

The infrastructure of the Institute (whether owned directly by IIC or accessible through cooperation with other parties) reflects the research topics of the IIC as determined by the national and international projects undertaken. The modernized infrastructure has allowed successful accomplishment of certain scientific tasks from a wide range of research categories: i) spectroscopy, ii) physico-chemical and thermo-chemical analysis, iii) preparation of ceramic, glass and other inorganic materials, and iv) characterisation of materials.

2.9. Supplementary information and/or comments on all items 2.1 – 2.8 (max. 2 pages in total for the whole section)

Human sources: Over the assessment period the policy of improving the qualification level of the research teams of the Institute was pursued by the following measures:

- Employing researchers who have worked abroad for a certain period and want to return.
- Employing PhD students that completed their thesis with us and they would like to continue their scientific career at our Institute.
- Employing excellent researchers as postdocs (e.g. through Euraxess) from Institute funds.
- Competing for various supporting grants of the Slovak Academy of Sciences (SASPRO, Morepro, Impulz, Doktogrant, Stefan Schwarz fellowship, support of young scientists).
- Competing for various national grants that provide short visits (e.g. SAIA) or enable employment for longer periods (e.g. APVV, 4 years).
- Competing for various international grants (e.g. from EU schemes).

The institute was active and successful in all of the activities just listed. It must however be noted that, in many cases, enormous administrative obstacles need to be overcome. Probably the most complicated is the acceptance process from the Foreign Police Department (for people from non-E.U. countries). It often takes six months or even more to complete all the requirements for a researcher from a non-E.U. country to start work.

One of the important aspects is the **gender issue** of the Institute. The ratio of men:women among researchers was 32:14 in 2016, 26:16 in 2018, and 31:18 in 2021, and 39:36 for all employees in 2021. It is important to note that the Institute has put effort into creating positions for women in the management of the Institute. The following positions were occupied by women: head of the scientific board, head of two departments (Department of Hydrosilicates, Economy and Service Section) and the secretary of education, which results in a man:woman ratio of 11:5 for all management positions. We consider this ratio as a good achievement for an institution predominantly oriented towards technical science.

Personnel development: This topic is the most important issue for the development of the Institute. The key issue remains one of providing the conditions for the further career development of all researchers. These issues are e.g motivation for self-education, motivation to create new contacts, providing exchange of experiences and new ideas, integration into the international research scene, and presenting our results to leading consortia. Due to the lack of graduate students from the field of inorganic chemistry in Slovakia, we are trying to attract PhD students and post-docs from foreign countries to join the Institute as well; we are pleased to say that we have had some success so far.

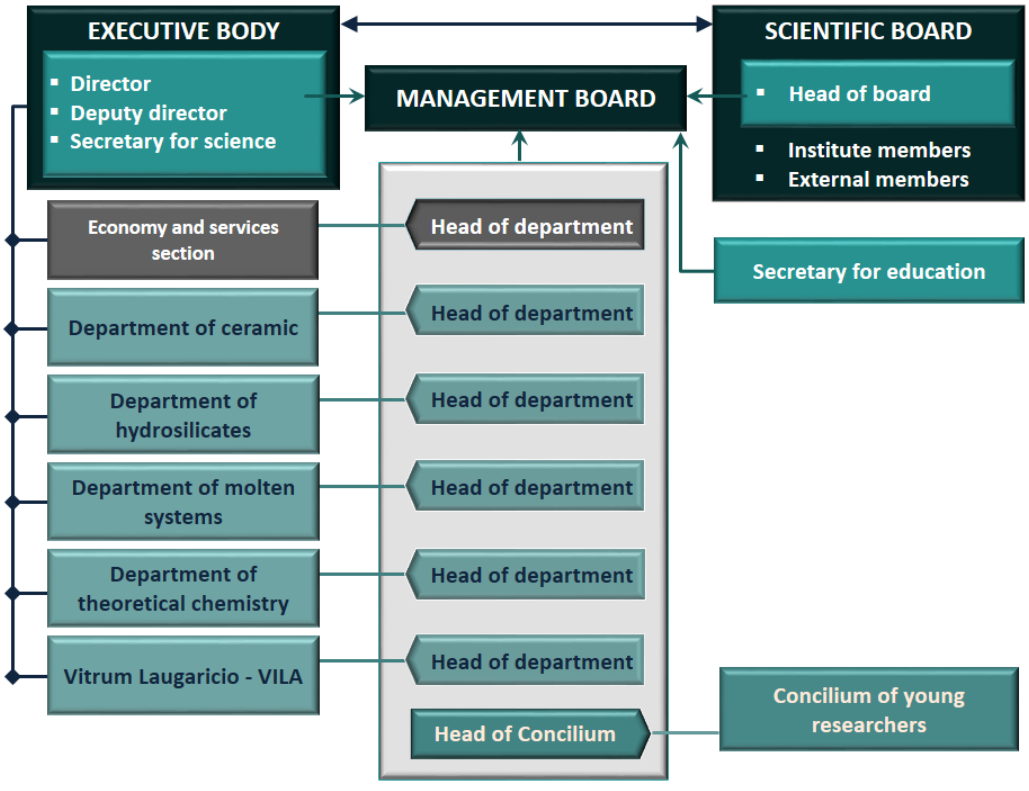
INTERNATIONAL MOBILITY - FOREIGN GUESTS AT IIC SAS

Country	Visits	Days spent at IIC
Austria	4	69
China	1	181
Czech Republic	10	63
Great Britain	2	279
Greece	1	93
India	1	91
Pakistan	1	91
Poland	4	62
Russia	3	121
Turkey	2	169
Ukraine	3	308
Overall	32	1527

32 visits to the Institute by researchers, including PhD students, were made during the years 2016-2021 within the frameworks of bilateral and multilateral projects, with an average length of 47 days.

The management of the Institute is well-defined and well-performed with clear competencies. However, it must be noted that many researchers are required to undertake administration, especially in relation to applying for structural funds. In order to involve young colleagues in management activities, a special body operates at the Institute – the Concilium of Young Scientists. Their representative actively participates in the weekly management meetings and they solve some specific problems independently with full responsibility (such as PR management of the Institute, and activities like Open Doors Day and Researchers' night).

Organisation structure of the IIC SAS:



3. Implementation of the recommendations from the previous evaluation period

- **The numbers of publications in highly cited international journals should be further increased.**

This task has been successfully addressed, as can be seen from the tables presented in 2.1.8:

- The average IF in 2015 was 2.27 – this was almost doubled in 2021!
- The number of publications has significantly increased in the last two years.
- Also, the median IF has trended u,p from 2.35 in 2015 to 3.65 in 2021 (more than a 50% increase).
- The proportion of publications in journals with higher IF has increased steadily, from a modal IF of 2-3 in 2015 to IF of 4 or more in the last three years. [See table in 2.1.8.]
- It is worth mentioning the list of publications with IF higher than 8:

1. BALTRUSAITIS, J. - BUČKO, Tomáš - MICHAELS, W. - MAKKEE, M. - MUL, G. Catalytic methyl mercaptan coupling to ethylene in chabazite: DFT study of the first C-C bond formation. In Applied Catalysis B: Environmental, 2016, vol. 187, p. 195-203. (8.328 - IF2015).
2. BUJDÁK, Juraj. The effects of layered nanoparticles and their properties on the molecular aggregation of organic dyes. In Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2018, vol. 35, p. 108-133. (15.325 - IF2017)
3. DRAČÍNSKÝ, Martin - BUCHTA, Michal - BUDĚŠÍNSKÝ, Miloš - VACEK-CHOCHOLOUŠOVÁ, Jana - STARÁ, Irena G. - STARÝ, Ivo - MALKIN, Oľga. Dihydrogen contacts observed by through-space indirect NMR coupling. In Chemical Science, 2018, vol. 9, no. 38, p. 7437-7446. (9.063 - IF2017).
4. REY, Jérôme - RAYBAUD, Pascal - CHIZALLET, Céline** - BUČKO, Tomáš**. Competition of secondary versus tertiary carbenium routes for the type B isomerization of alkenes over acid zeolites quantified by ab initio molecular dynamics simulations. In ACS Catalysis, 2019, vol. 9, no. 11, p. 9813-9828. (2018: 12.221 - IF, Q1 - JCR, 4.702 - SJR, Q1 - SJR, CCC).
5. REY, Jérôme - BIGNAUD, Charles - RAYBAUD, Pascal - BUČKO, Tomáš** - CHIZALLET, Céline**. Dynamic features of transition states for beta-scission reactions of alkenes over acid zeolites revealed by AIMD simulations. In Angewandte Chemie, 2020, vol. 59, no. 43, p. 18938-18942. (2019: 12.959 - IF, Q1 - JCR, 5.438 - SJR, Q1 - SJR, CCC).
6. VÍCHA, Jan - NOVOTNÝ, Jan - KOMOROVSKÝ, Stanislav - STRAKA, Michal** - KAUPP, Martin** - MAREK, Radek**. Relativistic heavy-neighbor-atom effects on NMR shifts: Concepts and trends across the periodic table. In Chemical Reviews, 2020, vol. 120, no. 15, p. 7065-7103. (2019: 52.758 - IF, Q1 - JCR, 20.847 - SJR, Q1 - SJR, CCC).
7. QIN, Zhengxing* - ZENG, Shu* - MELINTE, Georgian - BUČKO, Tomáš - BADAWI, Michael - SHEN, Yangfeng - GILSON, Jean-Pierre - ERSEN, Ovidiu - WEI, Yingxu - LIU, Zhongmin - LIU, Xinmei - YAN, Zifeng - XU, Shutao** - VALTCHEV, Valentin - MINTOVA, Svetlana**. Understanding the fundamentals of microporosity upgrading in zeolites: Increasing diffusion and catalytic performances. In Advanced Science, 2021, vol. 8, no. 17, p. 2100001-1-2100001-9. (2020: 16.806 - IF, Q1 - JCR, 5.388 - SJR, Q1 - SJR, CCC).
8. WANG, Quan - SHAHEEN, Sabry M. - JIANG, Yahui - LI, Ronghua - SLANÝ, Michal - ABDELRAHMAN, Hamada - KWON, Eilhann - BOLAN, Nanthi - RINKLEBE, Jörg - ZHANG, Zengqiang**. Fe/Mn- and P-modified drinking water treatment residuals reduced Cu and Pb phytoavailability and uptake in a mining soil. In Journal of Hazardous Materials, 2021, vol. 403, p.123628-1-123628-9. (2020: 10.588 - IF, Q1 - JCR, 2.034 - SJR, Q1 - SJR, CCC).
9. MAN, Yi - WANG, Bo - WANG, Jianxu** - SLANÝ, Michal - YAN, Haiyu** - PING, Li - EL-NAGGAR, Ali - SHAHEEN, Sabry M. - RINKLEBE, Jörg - FENG, Xinbin. Use of biochar to reduce mercury accumulation in Oryza sativa L: A trial for sustainable management of historically polluted farmlands. In Environment International, 2021, vol. 153, p. 106527-1-106527-11. (2020: 9.621 - IF, Q1 - JCR, 2.582 - SJR, Q1 - SJR, CCC).
10. RAMTEKE, D. - HUJOVÁ, Miroslava - KRAXNER, Jozef - GALUSEK, Dušan - ROMERO, Acacio Rincon - FALCONE, Roberto - BERNARDO, Enrico**. Up-cycling of ';unrecyclable'; glasses in glass-based foams by weak alkali-activation, gel casting and low-temperature sintering. In Journal of cleaner production, 2021, vol. 278, p. 123985-1-123985-7. (2020: 9.297 - IF, Q1 - JCR, 1.937 - SJR, Q1 - SJR, CCC).

There are also other **44 works** published in 2016-2021 in scientific journals with **IF 5-8**.

- **More university lectures could help to increase the interest of PhD students in the subject.**

The total number of hours in which our researchers are involved in the pedagogical process at universities has not changed much, but the structure has changed significantly compared to the previous period. The result is a much larger share of lectures and seminars being taught by our researchers, instead of laboratory exercises led by PhD students of our institute as in the past; on average there were 120 hours/year of lectures and seminars in the last 6 years, compared to 31 hours/year in the previous period, and there are now on average less than 40 hours/year of laboratory exercises, compared to 214 hours/year of laboratory exercises in the previous period.

A significant amount of effort was put into increasing the contact of our researchers with students at all levels of university education, starting from the Bachelors level, through the Masters, and even at the PhD level.

One part of this effort was the increased number of contracts with universities enabling IIC to serve as an external education institute. Currently, we have three such contracts – with the Slovak University of Technology (Bratislava), Comenius University (Bratislava) and Alexander Dubček University of Trenčín.

The highest degree of attention, in terms of education, is paid to PhD students, whose instruction is the primary educational activity of IIC. PhD topics are annually announced through several channels, including Academic Positions, Euraxess, Research Gate, embassies all over the world and intensive communication with our partners; annually, we send more that 50 letters of expression of interest in cooperation.

All these activities have had a positive impact on the education activities of IIC. We supervise both Bachelor and Master theses. Concerning PhD students, the number of candidates for PhD study increases annually. Thus, we have to select the suitable candidates in two runs; the first round is preselection in order to select candidates for the official selection round. Each year we have more candidates than the limit for PhD students. Thus, the effort for attracting PhD students as one of the IIC's priorities seems to be successful.

- **The institutes should aim at more funding at the EU level.**

In the evaluation period we participated in 13 submitted project proposals in various schemes including MSC, RIA and IA (see table below). Unfortunately, the success rate was rather small, only 15.4 %. We should submit more project proposals and become members of those working groups within EUMAT, EERA, SNETP which have fields of interest close to those studied at our institute. Moreover, if consortium is strong, we can apply for a project also in the field, where we do not have a long-term experience.

Acronym	Title	Call Identifier	Status
BEGEES	Beyond Lithium: Safe and efficient large-scale green electrochemical energy storage	H2020-LC-BAT-2019	Informed (Rejected)
SIMBA	Sodium-Ion and sodium Metal BAtteries for efficient and sustainable next-generation energy storage	H2020-LC-BAT-2020	Signed
ENERGY-TANDEM	Energy Tandem System	H2020-LC-SC3-2020-EC-ES-SCC	Informed (Rejected)
PPGD	Plasma-Pulse Geo-Drilling - A novel drilling technology to reach cost-effectively depths in the order of 5 km and/or temperatures higher than 250 deg C.	H2020-LC-SC3-2018-RES-TwoStages	Informed (Rejected)
DEEP-PPGD	Deep plasma power geo drilling	H2020-LC-SC3-2020-RES-RIA	Informed (Rejected)
CORMFS	Corrosion Mechanisms with Microstructure Damage for Ni-Based Alloys used in Molten Fluoride Salts	H2020-MSCA-IF-2016	Informed (Rejected)
SASAMA	VALORISATION OF CELLULOSE AND CLAY HIGHLY DISPERSED ON MIXED OXIDES MATERIALS FOR ELECTROCHEMICAL RECOVERY OF ACTINIDES AND LANTHANIDES IN MOLTEN FLUORIDE	H2020-MSCA-IF-2016	Informed (Rejected)

UltraCom	Development of New Ultra-High Temperature Ceramic Matrix Composites with Improved Oxidation/Ablation Properties for Aerospace Industry	H2020-MSCA-IF-2016	Informed (Reserve List)
CeramCom	New Generation Ultra-High Temperature Ceramic Matrix Composites for Aerospace Industry	H2020-MSCA-IF-2017	Signed
NGETMA	New generation of eco-friendly ionic liquids for highly efficient electrochemical treatment of metals and alloys	H2020-MSCA-IF-2019	Informed (Rejected)
ADVANTAGES	ADVanced nano-cerAmics for greeN and environmenTAl technoloGiES	H2020-MSCA-ITN-2016	Informed (Rejected)
ADVANTAGES	ADVanced nano-cerAmics for greeN and environmenTAl technoloGiES	H2020-MSCA-ITN-2017	Informed (Rejected)
ADVANTAGES	ADVanced nano-cerAmics for greeN and environmenTAl technoloGiES	H2020-MSCA-ITN-2018	Informed (Rejected)

- **Further possible connections to commercial applications should be explored.**

IIC won an international competition, set up by a consortium of the companies Rio Tinto and Hydro Aluminium, for development of a method for monitoring the quality of alumina used in aluminium production. IIC succeeded, even though facing high-level international companies like SINTEF, research group from Toulouse University or Light Metal Research Center (commercial shoulder of the University of Auckland) from New Zeland. On the basis of the results obtained, the consortium has decided to extend the contract for activities and research with IIC. This activity continues up to now and was extended for other topic like mesurements of electrical conductivity or characterisation of input flows.

From the point of view of the commercialization of the results, it will be necessary to examine possible collaborations with industrial partners, especially in the field of battery development and production. We are currently working intensively in this area, and we have already achieved interesting results. This explicitly falls into the category of applied research, where the commercialization of our results is expected.

Another area of our research with great potential for commercial use is the development of cement-ceramic composites. In this case, it will be necessary to contact a manufacturer of traditional building ceramics (a brickyard), who would help us to verify the laboratory results under the conditions of mass production.

The results achieved in the field of development of ultra-high-temperature diboride-based systems are also noteworthy. These are new ceramic materials with properties that make them suitable for a wide range of applications. As an example, we are currently dealing with LEC GmbH in Austria in order to verify the potential of these materials for spark plugs.

Finaly, we provide also a list of cooperation as was stated in chapter 2.3.1.

Cooperation with industrial partners in Slovakia
Amec Foster Wheeler Nuclear Slovak Republic s.r.o. - supplier of industrial equipment in Jaslovské Bohunice
AT Crystals, s.r.o. Žilina – company for research and experimental development in the natural and technical sciences
BEKAERT HLOHOVEC, j.s.c., Hlohovec - manufacturer and supplier of steel wire and cord
CEIT Technical Innovation, s.r.o. - member of CEIT group, Žilina
CONFAL, j.s.c., Slovenská Ľupča – company for recycling of aluminium
Golde Lozorno spol. s r.o. (Inteva Products Slovak Republic spol. s r. o.) - manufacturer of car parts
Hanon Systems Slovak Republic s.r.o. Ilava - manufacturer of car parts
KONŠTRUKTA - Defence, a.s Dubnica nad Váhom - development and testing of electronic systems
LB Minerals, j.s.c., Košice - a group member Lasselsberger, supplier of mineral resources
Malokarpatské múzeum v Pezinku - museum - history of viticulture
MICROWELL, spol. s r.o.Šaľa - measuring and control technology
Mikrochem spol. s r.o., Pezinok - pharmaceutical and chemical manufacturing company
Múzeum mesta Bratislavy - Museum of the City of Bratislava
PPC Čab, a.s - manufacture of porcelain insulators
Považská cementáreň Ladce, j.s.c., Ladce - cement production
RONA, j.s.c., Lednické Rovne – glass production company
Slovalco, j.s.c. Žiar nad Hronom – aluminium production company

TIMM Slovak Republic s.r.o.Trenčín - ropes manufacturer
VETROPACK NEMŠOVÁ s.r.o., Nemšová - container glass manufacturer
VUEZ, j.s.c., Levice - engineering, manufacturing, and installation company
VUJE, j.s.c., Trnava, an engineering company in the field of nuclear and conventional power generation
ŽSR, Bratislava - the largest passenger railway carrier in Slovakia

Cooperation with research institutions and universities in Slovakia
Centre for Advanced Materials Application (CEMEA), Slovak Academy of Sciences, Bratislava
Earth Science Institute, Slovak Academy of Sciences, Banská Bystrica
Faculty of Chemical and Food Technology, Slovak University of Technology, Bratislava - Department of Inorganic Technology
Faculty of Electrical and Information Technology, Slovak University of Technology, Bratislava - Institute of Nuclear and Physical Engineering
Faculty of Industrial Technologies in Púchov, The Alexander Dubček University of Trenčín - Department of Material Technologies and Environment
Faculty of Materials Science and Technology in Trnava, Slovak University of Technology - Institute of Materials Science
Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava
Faculty of Metallurgy, The Technical University of Košice
Faculty of Natural Sciences, Comenius University,Bratislava - Department of Inorganic Chemistry, Department of Physical and Theoretical Chemistry, Department of Geology of Mineral Deposits, Department of Mineralogy, Petrology and Economic Geology, Department of Engineerig Geology, Department of Microbiology & Virology
Faculty of Natural Sciences, University of Matej Bel, Banská Bystrica
Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava
Institute of Experimental Physics, Slovak Academy of Science, Košice
Institute of Materials and Machine Mechanics, Slovak Academy of Sciences, Bratislava
Institute of Materials Research, Slovak Academy of Sciences, Košice
Institute of Physics, Slovak Academy of Sciences, Bratislava
Institute of Virology BMC, Slovak Academy of Sciences, Bratislava
J. Selye University, Komárno
Polymer Institute, Slovak Academy of Sciences, Bratislava
The Alexander Dubček University of Trenčín - Central Laboratories, FunGlass
University of Žilina

Cooperation with industrial partners abroad
Austria
Aerospace & Advanced Composites GmbH., Austria - research, development and engineering of materials, technology and testing
LEC GmbH, Austria – development of ceramic materials for spark plugs
Lithoz, GmbH., Austria - development and production of ceramic materials and additive manufacturing systems (3D printing), ceramic prototypes, small scale series and complex parts
MAM Health & Innovation GmbH, Vienna, Austria - company for plastics product manufacturing
RHI AG, Technology Center, Standort Leoben, Austria - supplier of high-grade refractory products, systems and services for industrial high-temperature processes exceeding 1 200°C
RHP Technology GmbH, Austria
Belgium
Umicore Group R&D, Olen, Belgium
Canada
Elysis, Montreal, Canada
Czech Republic
Glass Service, a.s, Rokytnice, Czech republic – innovated services, hardware and software for improve glass melting, conditioning and forming efficency
UJV Řež Inc., 250 68 Husinec, Czech Republic
France
Rio Tinto Aluminium Pechiney, Voreppe, France
India
Evantes Trading Company, Bengaluru, India
Italy
Nuova Ompi, Padua, Italy - company for Manufacture of glass and glass products
Norway
Norsk Hydro ASA, Oslo, Norway
Switzerland
Home Art & Sales Services AG, Wollerau, Switzerland
Turkey
Eczacibaşi-Monrol Nuclear Products Co., Istanbul, Turkey - nuclear medicine company
USA

Alcoa Technical Center LLC, New Kensington, USA
Diver Solar LLC, Albuquerque, USA

Cooperation with research institutions and universities in abroad
Austria
Austrian Research Center, Materials Science Division, Austria
Department of Chemistry and Physics of Materials Paris Lodron University of Salzburg, Salzburg, Austria
Materials Center, Leoben, Austria
Montan Universität, Leoben, Austria
University of Natural Resources and Applied Life Sciences, Vienna, Austria
University of Vienna, Faculty of Chemistry, Institute of Inorganic Chemistry, Vienna, Austria
Belgium
The University of Ghent, Department of Inorganic and Physical Chemistry, Belgium
Canada
Department of Chemistry, The University of British Columbia, Canada
China
Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, China
Northeastern University, Shenyang, China
Northwestern University, XiAn, China
Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai, China
Southwest Jiaotong University, Chengdu, China - School of Materials Science and Engineering
University of Chinese Academy of Sciences, Beijing, China
Czech Republic
Brno University of Technology, Czech Republic
CEITEC – Central European Institute of Technology, Masaryk University, Brno, Czech Republic
Centre of Polymer Systems, Tomas Bat'a University in Zlín, Zlín, Czech Republic
Faculty of Civil Engineering, Czech Technical University in Prague, Czech Republic - Department of Materials Engineering and Chemistry
Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic
Institute of Inorganic Chemistry of the AS CR, V.V.I., Czech Republic
Institute of Geological Sciences, Faculty of Science, Masaryk University, Brno, Czech Republic
Institute of Inorganic Chemistry of the AS CR, V.V.I., Czech Republic
Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, Czech Republic
Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic
Masarykova Univerzita Brno, Czech Republic
University of Chemistry and Technology, Prague, Czech Republic
Univerzita Pardubice, Czech Republic
VŠB-Technical University of Ostrava, Ostrava, Czech Republic
Denmark
Department of Chemistry, University of Copenhagen, Copenhagen, Denmark
France
Conditions Extremes et Materiaux: Haute Temperature et Irradiation, CNRS, Orleans, France
European Synchrotron Radiation Facility, Grenoble, France
Faculte des Sciences, Universite d'Orleans, Avenue du Parc Floral, BP 6749, 45067 Orleans cedex 2, France
Institut de Chimie des Milieux et Matériaux de Poitiers – IC2MP, UMR CNRS, Université de Poitiers, France
Institut de Chimie Moléculaire de l'Université de Bourgogne (ICMUB, UMR CNRS 6302), Dijon, France
Institut des Molécules et des Matériaux du Mans, Université du Maine, Le Mans, France
University of Lyon, France
Université de Toulouse, Laboratoire de Génie Chimique, France
Germany
Fraunhofer Institute for Ceramic Technologies and Systems, Germany
Institute for Geosciences, Friedrich-Schiller-University Jena, Germany
Institute of Chemistry, Technische Universität Berlin, Berlin, Germany
Institute of Technical Thermodynamics DLR, Germany
Joint Research Centre for Nuclear Safety and Security, European Commition, Karlsruhe, Germany
Karlsruhe Institute of Technology, Germany
Technische Universität Darmstadt, Darmstadt, Germany
Universität Bayreuth, Germany
Greece
Department of Geology, University of Patras, Patras, Greece
Department of Mechanical Engineering, University of the Peloponnese, Patra, Greece
Hungary
Faculty of Science and Informatics University of Szeged, Szeged, Hungary
Italy
Dipartimento di Chimica, Università di Torino, Torino, Italy
ENEA Research Centre, Casaccia, Italy
Institute for Ceramic Technology, ISTEC, Faenza, Italy

Politecnico di Torino, Torino, Italy - Department of Applied Science and Technology
The University of Trento, Materials Science Department, Trento, Italy
Universita di Padova, Dipartimento di Ingegneria Industriale, Italy
Japan
Advanced Institute for Materials Research (AIMR) Tohoku University, Sendai, Japan
Interdisciplinary Graduate School of Science and Engineering, Shimane University, Matsue, Japan
National Institute for Advanced Industrial, Science and Technology (AIST), Nagoya, Japan
National Institute for Materials Science, Tsukuba, Japan
Norway
Department of Materials Science and Engineering, Norwegian University of Science and Technology, Norway
Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, UiT–The Arctic University of Norway, Tromsø, Norway
Poland
AGH University of Science and technology, Krakow, Poland
Faculty of Chemistry, University of Warsaw, Warszawa, Poland
Institute of Fundamental Technological Research, Polish Academy of Science, Warsaw, Poland
Institute of Organic Chemistry, Polish Academy of Sciences, Warszawa, Poland
Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Krakow, Poland
Russia
Department of Rare Metals and Nanomaterials, Institute of Physics and Technology, Ural Federal University, Ekaterinburg, Russia
G. K. Boreskov Institute of Catalysis, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia
Institute of Chemistry and Technology of Rare Elements and Mineral Raw Materials, Kola Science Centre RAS, Russia
Sobolev Institute of Geology and Mineralogy, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia
Tanatnaev Institue of Chemistry, Kola Science of Russian Academy of Sciences, Apatity, Russia
Ural Federal University, Department of Theoretical Physics and Applied Mathematics, Ekaterinburg, Russia
Serbia
Faculty of Technology, University of Novi Sad, Serbia
University of Novi Sad Faculty of Technology, Serbia
Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia
Slovenia
Jožef Stefan Institute, Engineering Ceramics Department, Ljubljana, Slovenia
Spain
Instituto di Cerámica y Vidrio, Madrid, Spain
University of the Basque Country, Departamento de Química Física, Bilbao, Spain
Taiwan
National Cheng Kung University, Taiwan - Department of Material Science and Engineering
National Taiwan University of Science and Technology, Taipei, Taiwan
Turkey
TUBITAK Marmara Research Center, Materials Institute, Barış Mah, Turkey
Ukraine
Ukrainian State University of Chemical Technology, Dnipro, Ukraine
United Kingdom
EaStChem School of Chemistry, University of St Andrews, St Andrews, UK
Queen Mary University of London, London, United Kingdom
USA
Department of Biological, Chemical and Physical Sciences, Roosevelt University, Chicago, Illinois, USA
Lehigh University, Department of Chemical and Biomolecular Engineering, Betlehem, USA
The University of Alabama, Tuscaloosa, USA
University of Illinois, Champaign-Urbana, USA
University of Minnesota Duluth, USA
University of Wisconsin-Madison, Madison, USA
Valparaiso University, Valparaiso, USA

Cooperation with educational partners in Slovakia
All4Science, o.z., Chorvátsky Grob

4. Research strategy and future development of the institute for the nextfive years (Recommended 3 pages, max. 5 pages)

Research strategy of the institute in the national and international contexts, objectives, and methods (including the information on when the strategy was adopted)

Our fundamental and primary goals, to which all aspects of the Institute's activities should be aimed, are: professional growth, international integration and the societal benefits of research results. We want to:

- be a dignified and respectable research partner,
- participate in the further development of the key scientific fields which the Institute was established for and has accumulated significant experience in,
- be a part of the broader multi-disciplinary scientific community.

Our vision is to achieve a state where our Institute will be sought out as a centre of international cooperation on important topics with the possibility of training young scientists. More specifically for each department:

Department of Ceramics:

Based on research experiences and achievements in the past, the following key research topics have been selected by the Department of Ceramics for the near future:

1. Energy conversion and storage: In the past, the main emphasis was on the research and development of nitride- and oxynitride-based photoluminescent materials (powders) for LEDs and thermoelectrics. Recently, the research has become more oriented toward the development of translucent/transparent phosphors for high power LEDs and/or materials for photocatalytic applications in waste water and air cleaning. Since 2019, we have started to work on the development of ceramic materials for the new generation of batteries. The currently investigated topics are the following: 1) Development of an anode for Li-ion batteries based on carbon-silicon composites (APVV-19-0461), 2) Sodium-ion and sodium metal batteries for efficient and sustainable next-generation energy storage (H2020), and 3) Porous ceramic anodes for next-generation sodium batteries (VEGA-0167-22).
2. Bioceramics: Within this topic, the main research activities are focused on silicon nitride-based ceramics, which form a new type of bio-ceramic material when combined with a bio-active additive (e.g. hydroxyapatite). So far, we have succeeded in preparing a composite ceramic biomaterial with a defined porosity, which resembles trabecular bone in terms of structure and mechanical properties. The developed materials meet various application requirements, e.g. those for bone implants. Currently the research is focused on: 1) Development of bio-active silicon nitride by surface layer modification (APVV-18-0542, TUBITAK, VEGA-0161-22); 2) Preparation and characterization of granules / microspheres based on silicon nitride for bio applications; 3) Nano-structured, functionally-layered and bio-inspired 3D implants based on titanium (APVV-20-0322);
3. New technologies and materials: The main goal is to develop new advanced ultra-high temperature ceramics (UHTC) and high-entropy ceramics (HEC) with improved properties at very high temperatures (above 2000°C). In addition, current research activities are also focused on the combination of UHTC with ceramic matrix composite materials (CMC) to develop new so-called ultra-high-temperature ceramic matrix composites (UHTCMC). The application potential of these materials in aerospace and nuclear industries will be significantly enhanced by the development of an appropriate technique to join them to similar or dissimilar materials. The most recent research topics are the following: 1. Development of refractory pyrochlore phases for high-temperature applications of non-oxide ceramics (APVV-17-0378); 2. New high-entropic ceramic materials for advanced applications (APVV-19-0297); 3. Electromagnetic shielding of functionally-gradient-layered composites based on SiC with the addition of graphene and carbon nanotubes (VEGA-2-0007-22).
4. Utilisation of domestic raw materials and wastes: The aim is to provide added value to the domestic raw material base (magnesite, dolomite, etc.), and to address various options for the

recovery of wastes as secondary raw materials for the preparation of advanced or refractory ceramic and glass-ceramic materials based on oxides, carbides and oxynitrides. As these are high-tonnage raw materials and wastes, their main use is anticipated in civil engineering (aggregates, aerated concrete, bricks, etc.).

Department of Hydrosilicates:

The research in the Department of Hydrosilicates in the near future will be aimed at completing tasks planned in ongoing national scientific projects. Four national projects are currently underway, which will be completed over the next four years, with another project starting in 07/2022. The topics of these projects relate to current modern research trends, but all share a common research subject – layered silicates. The successful completion of each of the projects requires knowledge, skills and know-how in the chemistry of layered silicates from the smectite group, as well as their chemical modifications.

1. The primary topic in the next few years will be composite materials with unconventional modifying substances – cationic and non-ionic polymers (APVV-19-0487; VEGA 2/0166/21). A similar approach was successfully used in recent years by our group in research that focused on incorporation of non-commercial surface-active substances, such as quarternary alkylammonium and phosphonium cations, into clay minerals as modifications, and to use them in preparation of polymer/clay nanocomposites. In contrast to previous years, the emphasis will be on the design of bionanocomposites or materials which are non-toxic or even biocompatible. Our long-term collaboration with the Polymer Institute of the SAS in this field is a good example of effective national research within the SAS. This cooperation resulted in common projects and publications and it is expected that this will continue in the following period.
2. A second significant line of research will be the preparation of multicomponent systems based on modified clay minerals or polymer membranes together with active molecules which will impart photosensitizing, antibacterial and luminescent properties to the resulting materials (APVV-18-0075; APVV-21-0302). The main part of this research will be the preparation of ternary systems of layered silicates, in which dye molecules represent the components possessing the desired functionality of the materials. This area has been under development for a while, with several successfully completed projects already, and future work is planned to include materials with antimicrobial surfaces. The characterization of the materials will be carried out in cooperation with the Faculty of Natural Sciences of Comenius University in Bratislava. The main contribution of the team will be to design suitable hybrid materials with desired optical properties, and predicting which silicate carrier to choose for specific types of hybrid material and which surface modification should be carried out in order to obtain specific material properties or applications.
3. In the last year, new environmental topics involving adsorbents based on clay minerals from Slovakia (APVV-20-0175) have begun to be developed in the department by young researchers, and this will continue in the next few years. Several research institutes collaborate with our group, mainly in the EU and Japan, providing know-how and infrastructure for special research methods. Presently, the department team consists of four promising young researchers under the age of 35, and two in the age range of 35-40 years. We are also happy to report that, for at least the next three years, the team will be enriched with another researcher, who has successfully applied for a position under the SASPRO project scheme.

Department of Molten Systems:

1. In the field of metal extraction, our approach to enhancing metal recovery and sustainability consists of operating the separation directly at the reduction step using electricity. In this context, we are currently investigating the development of a new electrochemical route for metal production in extreme environments. The principle of this process is to extract the elements individually or in the form of alloys in the molten state in an electrolysis cell with molten salt electrolytes, in order to replace the existing capital-intensive and environmentally-harmful operations. The goal will be to offer a set of physicochemical data on the new molten salt electrolytes such that the data can be used to better facilitate physical, chemical, and economic assessments of the new industrial electrowinning processes. It will focus on the need for a thorough analysis to understand, predict and optimize the physical properties of the molten fluoride systems that could be used in new electrolytic productions of metals, and obtain the data

necessary to support industrial reactor design/development. In the upscaling phase of new processes, significantly more in-depth modelling becomes very important for ensuring the design of an economic process, and the relevant physicochemical data of these electrolytes will be thus truly essential.

2. One important area of present inorganic chemistry is the search for new materials suitable for innovative electronic applications (solid-state ionics for solid electrolytes, and electronically-conductive materials for inert electrodes). This has led to the synthesis of a number of solid electrolytes with high conductivity due to various ions, in particular monovalent alkali-metal cations. Many investigations have focused on the structure and nonstoichiometry of the various compounds containing monovalent cations, especially Li and Na. Vacant sites in these structures give rise to extreme mobility of the monovalent cations, resulting in high values of two- and three-dimensional ionic conductivity The size and the role of the cations is also a key factor for understanding the transport properties of solid conductors. To understand the unusually high transport ability of alkali metal ions requires more rigorous characterization of the phases and those systems and subsystems where these phases and compounds arise and exist. The problem is that information about the relevant phases (in the form of phase diagrams) is rather limited, and likewise the thermal stability of all compounds contained in these systems. All of the studied alkali metal oxo-, fluoro-, and oxo-fluoro-complexes are examined as part of binary $MF-N_2O_3$ systems (M = alkali metals, N = Al, Sc, etc.), and these systems can be present as subsystems of wider reciprocal systems, e.g. $MF-AlF_3-N_2O_3-M_2O$. Rigorous understanding and characterization of these reciprocal systems could also be important to other industrial applications (e.g. glass chemistry, molten salt electrolytes for electrowinning of metals, luminophores, scintillators, etc.), so in addition to the primary scientific reason for this proposal (materials for solid electrolytes), a complete analysis of these systems will also be valuable for the broader scientific and industrial community in other ways.
3. We have applied for a Horizon Europe project through the Pathfinder scheme with the aim of developing a versatile battery system with an internal charger based on the breakthrough concept of a molten salt liquid rotor, capable of providing power simply when set to circulate. Our proposed system will use molten salts with suspended magnetic micro-particles as the medium for a liquid rotor in an electro-generator, with the possibility of using the same melt as a medium for energy storage. In particular, the thermal energy could be stored in molten-salt tanks, while the electrical energy storage would be tailored to the system's usage conditions (thus, it could be conventional batteries or molten-salt batteries). We plan to study this topic even in the case of non-supporting decision from EU.
4. It is desirable to continue systematic research on the ternary fluorides of lanthanides and other critical elements (listed by European Commission as critical materials for EU industry) to their extensive application potential (e.g. in electro-applications like components to electronics, sensors or even batteries or in optical applications). The research comprises thermo-chemical, electro-chemical, physico-chemical, spectral and structural analysis.

Department of Theoretical Chemistry:

The scientific strategy of the department stands on three pillars: 1) development of new computationally-efficient methods for relativistic and non-relativistic quantum-chemical calculations of spectroscopic properties, with an emphasis on heavy-element compounds; 2) development of theoretical tools for the analysis and interpretation of spectroscopic parameters in order to provide a deeper understanding of the observed/calculated trends; 3) application of newly-developed and already-available quantum-chemical approaches to practical problems that are of interest in a broad spectrum of scientific fields.

1. The key for establishing the first pillar is the implementation of the developed methods in quantum chemical packages available to the general (not only scientific) community. Here we first of all plan to continue improving our in-house program ReSpect, though development of other quantum-chemical programs is not excluded (*e.g.* VASP or Dirac). In particular, we plan: a) to develop a new generation of eXact 2-Component methodologies (X2C) for calculation of EPR, NMR, and electron absorption spectroscopies; b) to release new public versions of the ReSpect program on a two-yearly schedule starting in 2022; c) to improve the tutorials and manuals on the program at http://respectprogram.org/; d) to add an interactive interface on the webpage to process raw data from the ReSpect program (e.g. transform the outputs of the TDDFT module so

as to plot the UV-Vis or X-ray spectra from them); e) to release a version of the ReSpect binaries with a hybrid OpenMP/MPI parallelization scheme using singularity containers of other techniques.

2. We plan to continue working on extending the set of interpretative tools available in the ReSpect program. Our foreign partners who use the ReSpect code have already found them very beneficial in studying chemical problems of practical interest. However, there is a great potential for exploring a variety of approaches developed earlier for the non-relativistic analysis of spectroscopic properties of light-element compounds, and transferring some of them to the relativistic domain to study heavy-element compounds.
3. We will pursue the application of theoretical methods in collaboration with our foreign partners and within the institute. We have extensive experience with the former, whereas there is room for improvement in the latter. Strengthening the internal collaboration within the institute will necessarily expand the know-how and skills of the institute, which will further improve its competitiveness in the international context. A successful story of international and local (within the institute) collaboration is the Visegrad Group (V4)–Japan Joint Research Program on Advanced Materials [https://atomdec.info/]:

   Description of the project: Ab initio DFT calculations have confirmed the desirable properties of hybrid materials based on clay mineral, which make them usable in green technologies and competitive with the more expensive adsorbents, e.g. those based on graphene/graphene oxide. Comparative studies of both types of advanced materials are thus a big challenge for future theoretical studies and international collaboration in this field, since these materials have so far been studied individually and not in direct comparison. Furthermore, a new multilateral project among Japan and the V4 countries on the new carbon materials began in 2021. The calculations will help design new structures usable, e.g., in the field of supercapacitors, providing further details about the properties of these advanced materials and saving expensive measurement time, as well as saving chemicals for the synthesis of test systems (thus contributing to the health of the environment).“

Joint glass centre Vitrum Laugaricio (VILA):

VILA is a joint laboratory of IIC SAS, TnUAD, and FChPT STU, with its registered office in Trenčín, Slovakia. Both IIC SAS and TnUAD employ researchers on site. VILA uses the premises of TnUAD and IIC SAS contributes to the operating costs. In the organizational context of TnUAD, VILA is organized as a department of the Centre for Functional and Surface Functionalized Glasses (FunGlass), the only H2020 funded Teaming centre in the Slovak Republic. The following benefits result from this arrangement:

- Lower operating costs of the center for IIC SAS,
- Synergies resulting from cooperation with colleagues from TnUAD within VILA, as well as with colleagues from other FunGlass departments,
- Utilization of the experimental facilities of FunGlass,
- Exeptional publishing outputs and a higher success rate in obtaining research funding from domestic grant agencies,
- Access to doctoral students from TnUAD.

The scientific focus of the department is defined by the head of the department, in line with the scientific focus of the IIC SAS, on the basis of feedback from department staff and in accordance with their professional orientation, and also in line with the latest developments in the field.
The main research topics of the department in the immediate future are defined as follows:

- Bioactive glasses doped with elements with a potential therapeutic effect, plus studying of the kinetics of their degradation in body fluids in relation to their structure,
- Corrosion of glasses and ceramic materials in aqueous media,
- Development of new types of oxide ceramics, especially ceramics with eutectic microstructures and high entropy ceramics,
- Low-temperature sintering processes, such as cold sintering.
- Transparent polycrystalline ceramic materials doped with optically active elements.

The VILA management will be based on the principles of freedom of scientific research, project-oriented management, formation of ad-hoc teams solving specific R&D tasks with continuous control

of achieved results, and the support of collaboration with other departments of IIC SAS and FunGlass.

As can be seen from the state of research described by the individual departments, the Institute is aware of its position in the international research area as well as of its weaker aspects. Additionally, the following measures are planned in order to attain the aims defined above.

1. Progressive management of human resources
   - To focus attention on the career development of all categories of scientists, from PhD students up to senior researchers.
   - To encourage colleagues to create new contacts and go for both short and longer stays in laboratories abroad.
   - To maintain a desirable age balance of the staff.
   - To maintain the continuous training of the staff, including PhD students, in new methods and new research fields.

2. The following research areas are to be a primary focus:
   - Materials for energy applications: this covers research activities across all departments, including ceramic materials for lighting and new types of batteries, and corrosion tests in highly aggressive molten fluorides.
   - Biomaterials / Materials for health care: this covers mostly ceramic biomaterials and clay-based hybrid materials with antibacterial properties.
   - New technologies: ceramic technology for the preparation of the materials for extreme environments.
   - Domestic raw materials: exploitation of 1) magnesite for new applications, 2) inorganic waste, 3) clay minerals modified with specific organic surfactants for polymer clay nanocomposites.
   - Other functional materials: e.g. optical materials, including materials with luminescent properties; materials with electric or magnetic properties; structural glass-based materials; hybrid systems based on organic dyes and layered silicates.

3. Cooperative projects
   - To increase the Institute's participation in large international projects, financed from the European Commission or other sources outside Slovakia.
   - To support the creation of both domestic and international interdisciplinary research consortia.
   - To find methods and funding to accept post-docs from abroad.
   - To increase involvement in the research with industrial partners.
   - To continuously increase the quality of publications.

4. Infrastructure
   - To develop and upgrade our infrastructure in order to have laboratories providing both standard and specialised services.

The above measures define the research strategy of the Institute in the national and the international context. However, one important fact has not yet been mentioned. While each department solves certain specific problems, strong cooperation between departments is essential for the Institute's success. It must be emphasised that significant effort is put into ensuring cooperation between Institute departments. The departments participate together in joint projects, both academic and industrial, and have joint publications, and some specific measurement services performed by particular departments are provided for all researchers of the Institute.
It is essentially impossible to provide an exact time schedule for these strategies, as they strongly depend on governmental budget and other external factors. Nevertheless, we firmly intend to reach the defined aims and we hope they will be achieved during the next four-year evaluation period, at least to a substantial extent.

"Our vision is born from our mission but must be grown by our ambition."

M. Boča