INSTITUTE OF INORGANIC CHEMISTRY SAS

Assessment period 2012-2015

CONCEPT / PURPOSE

Assessed aspects

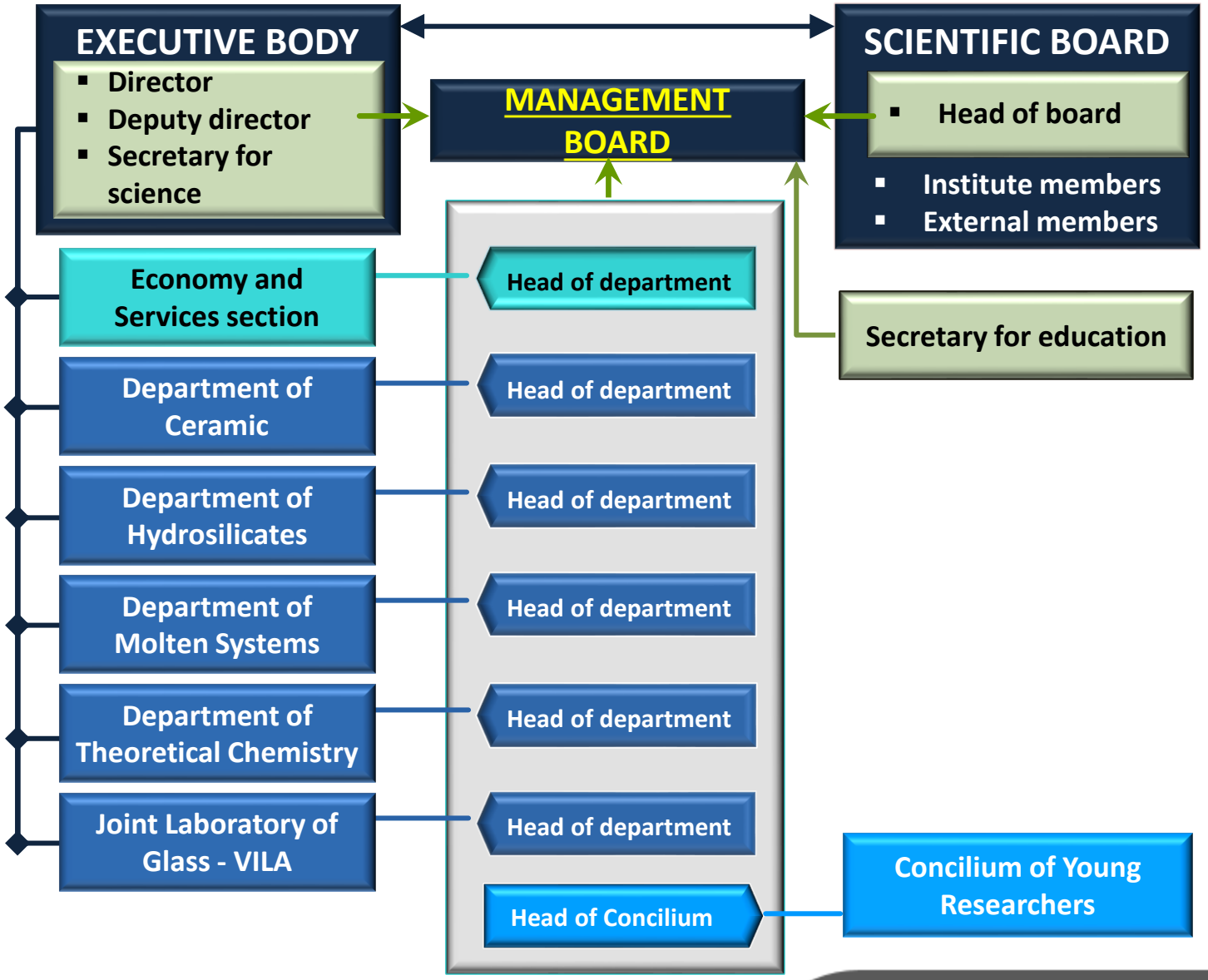
1. Scientific quality and productivity
2. Societal, cultural, and/or economic impact
3. Future prospects (development potential)

Questionnaire content

1. Basic information on the Institute
2. Partial indicators of main activities
3. Research strategy and future development plans of the Institute for the next five years (2016-2020)
4. Other information relevant to the assessment

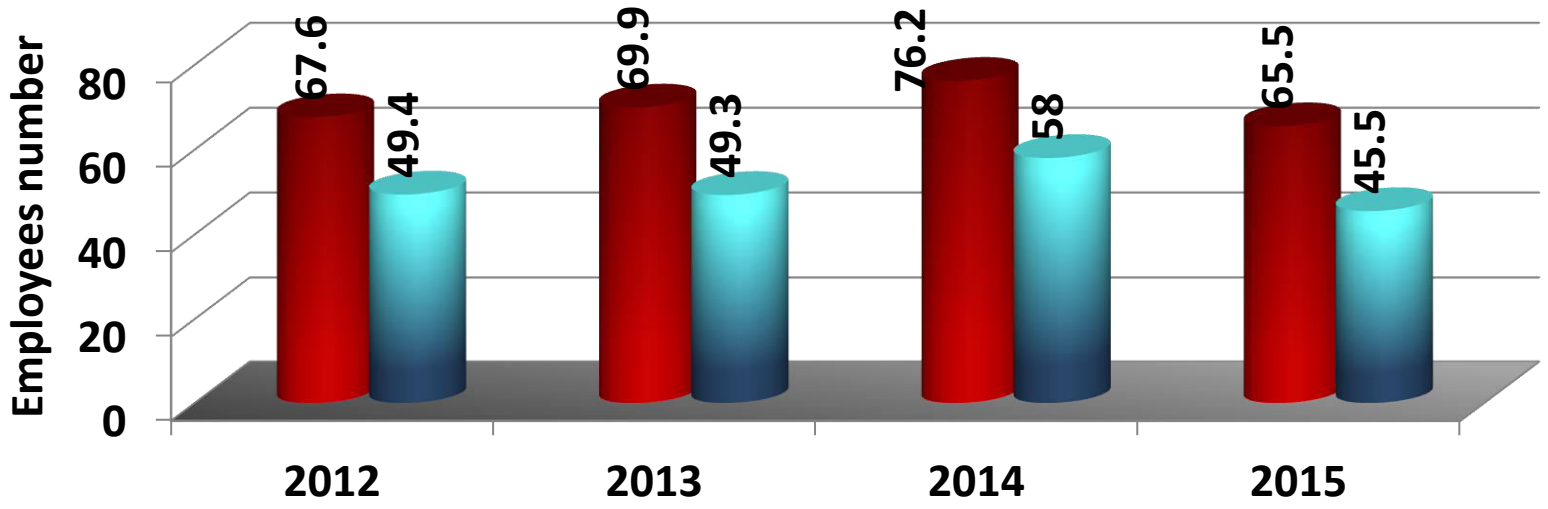
1. scientific outputs of Institutes;
2. feedback on scientific outputs of Institutes;
3. scientific status of Institutes in the international and domestic context;
4. project structure, grant and other financial sources;
5. postgraduate studies and other educational activities;
6. contribution to societal practice;
7. popularization of results;
8. environment and management: infrastructure, personal development.

1. Organisation structure of the Institute



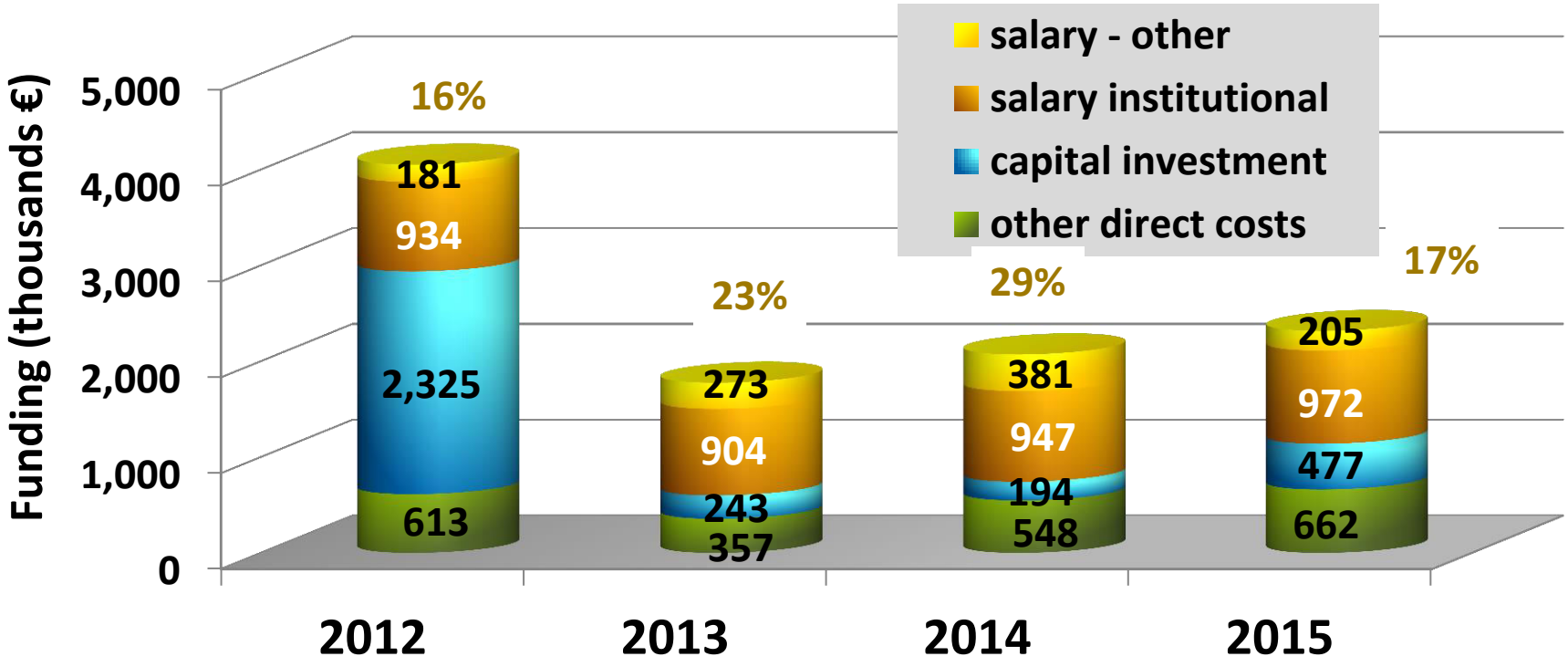
1. The Institute staff

- full time equivalent work capacity of all employees (state on 31.12.)
- full time equivalent work capacity of employees with university degrees engaged in research projects (state on 31.12.)



Ratio of researchers %	73	71	76	69
Average age	42.7	43.3	43.5	44.1

1. Basic information on funding

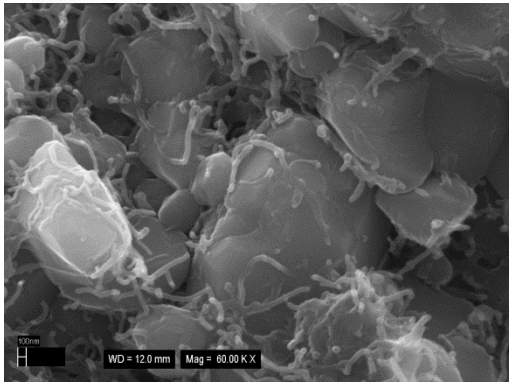


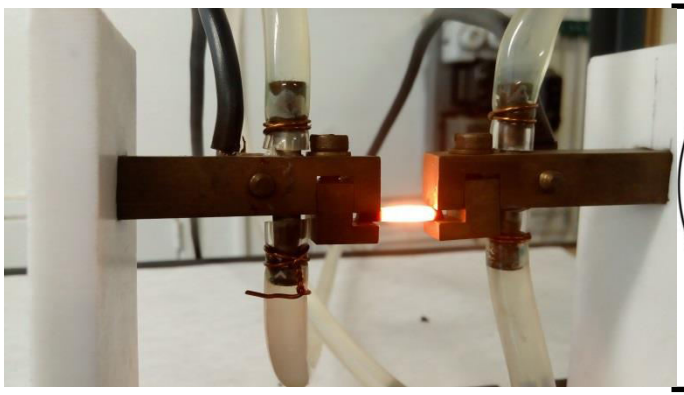
	2012	2013	2014	2015
Overall costs (thousands €)	4 052	1 776	2 071	2 316
Salaries (thousands €)	1 115	1 177	1 328	1 177

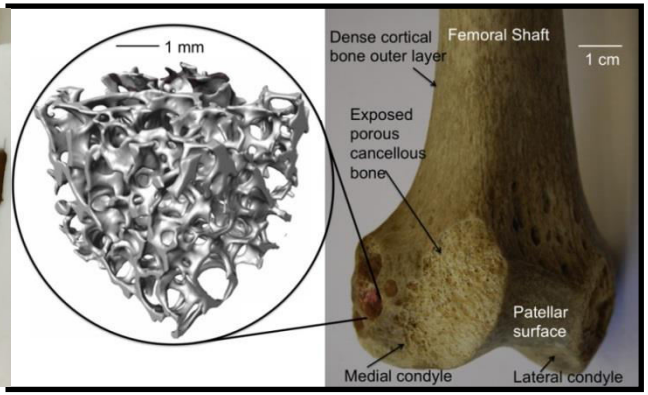
1. Research highlights – Department of Ceramic

Fields of interest:

- Microstructural design of new types of nano-composites (CNTs, graphene)
- Ceramic composites with high thermal and/or electrical conductivity
- Ceramic materials for solid state lighting
- Ultra-high temperature ceramic materials (borides, carbides)
- Bioceramics

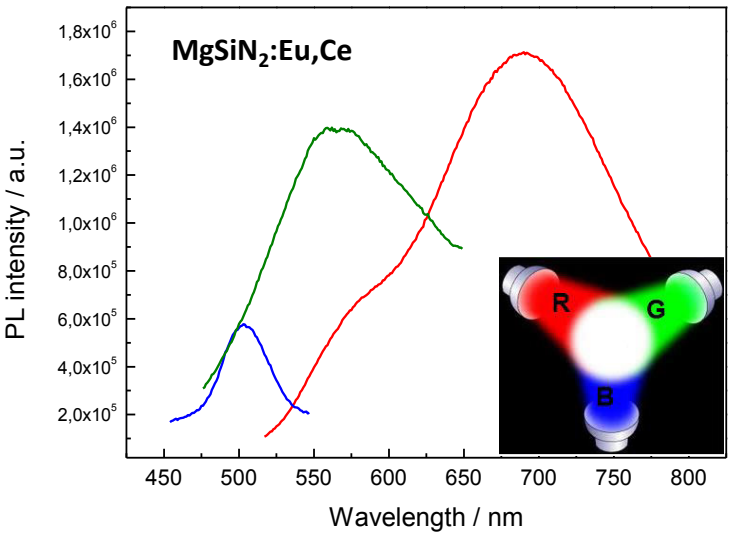






1. Research highlights – Department of Ceramic

Theoretical and experimental approach to solid state lighting



Projects:

- FP7-Marie Curie Initial Training Networks "Functional nitrides for energy applications" (FUNEA); (2011-2015)
- APVV-14-0385 Silicon oxynitride-based photoluminescent ceramic materials (2015-2019)

Japanese Patent

K. Hirao, Y. Zhou, Z. Lenčéš: Preparation of nitride phosphors by combustion synthesis, No. 5077930, (7.9.2012)

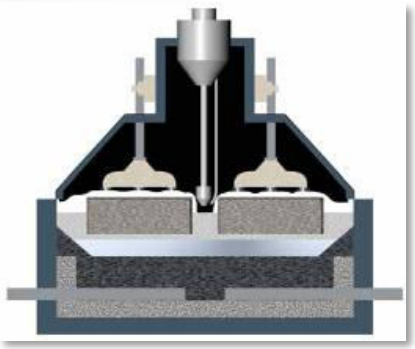
Publications:

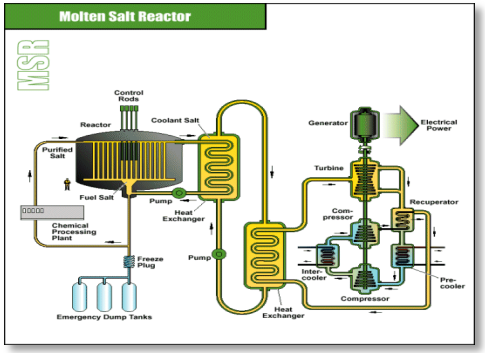
- Z. Lenčéš, M. Hrabalová, A. Czímerová, P. Šajgalík, Y. Zhou, K. Hirao, Luminescent properties of europium-doped lanthanum silicon nitride phosphor, J. Korean Ceram. Soc. 49, 325-327 (2012).
- I.A.M. Ibrahim, Z. Lenčéš, L. Benco, M. Hrabalová, P. Šajgalík, Cerium-doped $LaSi_3N_5$: computed electronic structure and band gaps. J. Eur. Ceram. Soc. 34, 2705-2712 (2014).
- I.A.M. Ibrahim, Z. Lenčéš, L. Benco, M. Hrabalová, P. Šajgalík, Samarium-doped $LaSi_3N_5$: synthesis, computed electronic structure and band gaps. J. Am. Ceram. Soc. 97, 2546-2551 (2014).
- I.A.M. Ibrahim, Z. Lenčéš, P. Šajgalík, L. Benco, M. Marsman, Electronic structure and energy level schemes of RE^{3+}:$LaSi_3N_5$ and RE^{2+}:$LaSi_3N_{5-x}O_x$ phosphors (RE = Ce, Pr, Nd, Pm, Sm, Eu) from first principles, J. Lumin., 164, 131-137 (2015).

1. Research highlights – Department of Molten Systems

Fields of interest:

- **Research of molten salts properties: fluorides, nitrides, chlorides**
  - **Physico-chemical analysis and calorimetric measurements** - viscosity, density, surface and interface tension, thermal analysis, electrical conductivity, ...
  - **Structural and spectral analysis** - XRF, X-ray and neutron diffraction, rapid solidification processing, solid state and high temperature NMR spectroscopy, ...
  - **Corrosion analysis** - for use in solar heat accumulation, nuclear powers or metal production

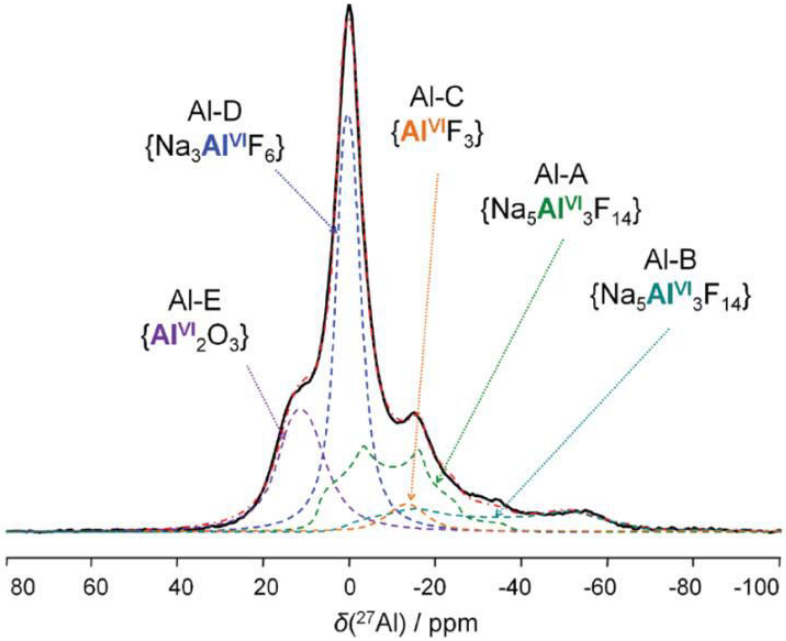




1. Research highlights – Department of Molten Systems

Application of modern spectral methods on fluoride systems

- HT and MAS NMR – identification of mechanism of oxides dissolution in basal melts
- XPS spectroscopy – development of new method for identification of different bonding modes of fluorine atoms



^{27}Al MAS NMR spectra of mixture Na_3AlF_6 - 10 mol% FeO

Publications

- M. Boča, P. Barborík, M. Mičušík, M. Omastová X-ray photoelectron spectroscopy as detection tool for coordinated or uncoordinated fluorine atoms demonstrated on fluoride systems NaF, K_2TaF_7, K_3TaF_8, K_2ZrF_6, $Na_7Zr_6F_{31}$ and K_3ZrF_7. Solid State Sciences 14, 828-832 (2012).
- M. Boča, A. Rakhmatullin, J. Mlynáriková, E. Hadzimová, Z. Vasková, M. Mičušík, Differences in XPS and solid state NMR spectral data and thermo-chemical properties of iso-structural compounds in the series $KTaF_6$, K_2TaF_7 and K_3TaF_8 and $KNbF_6$, K_2NbF_7 and K_3NbF_8. Dalton Trans. 44, 17106–17117 (2015).
- F. Šimko, A. Rakhmatullin, C. Bessada, and M. Boča, MAS NMR Study of the Solidified Cryolite Systems with FeO Addition. Journal of Fluorine Chemistry 165, 116-122 (2014).

Projects

- Inorganic fluoride melts – the complex study of spectral, diffraction, physico-chemical, thermodynamic and structural characteristics. APVV-0460-10; 2011-2014
- Molten fluoride systems for high temperature applications with potential in energy sector application. VEGA 2/0095/12; 2012-2015

1. Research highlights – Department of Hydrosilicates

Fields of interest:

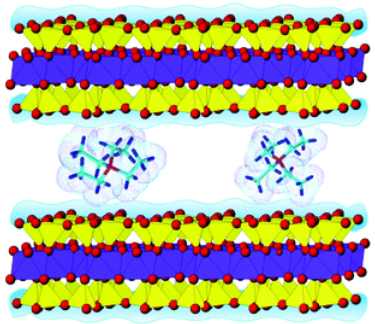
Natural clays / clay minerals

- Complex analysis
- Structural characterization
- Chemical modifications

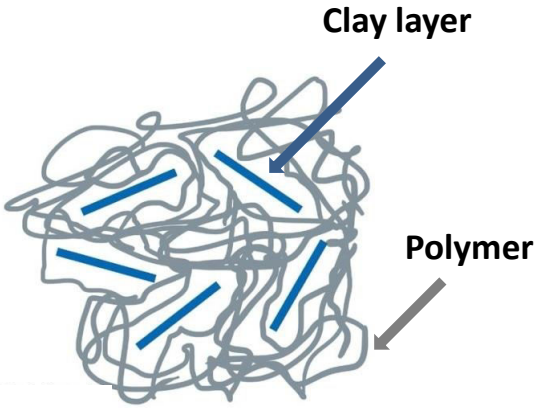
Clay deposit – Jelšový potok

Complex systems

- Hybrid materials based on organo-modified clay minerals
- Clay-polymer nanocomposites
- Photoactive materials with organic dyes



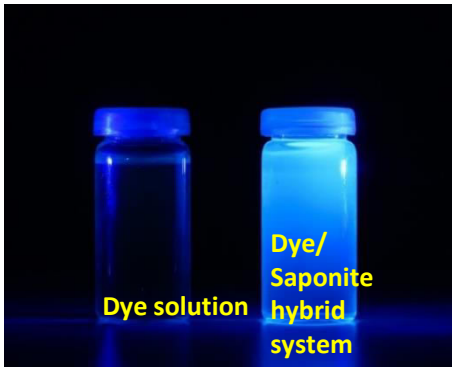
Organoclay

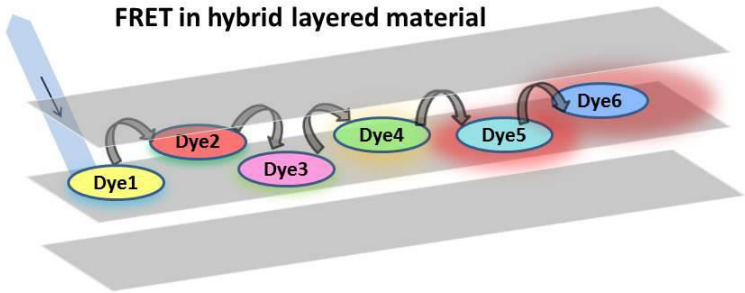


Clay-polymer nanocomposite

1. Research highlights – Department of Hydrosilicates

Photoactive materials with organic dyes





Publications

- J. Bujdák, Layer-by-layer assemblies composed of polycationic electrolyte, organic dyes, and layered silicates. Journal of Physical Chemistry C, 118, 7152-7162 (2014).
- P. Boháč, A. Czímerová, J. Bujdák, Enhanced luminescence of 3,3'-diethyl-2,2'-thiacyanine cations adsorbed on saponite particles. Applied Clay Science 127-128, 64-69 (2015).
- S. Belušáková, K. Lang, J. Bujdák, Hybrid systems based on layered silicate and organic dyes for cascade energy transfer. Journal of Physical Chemistry C, 119, 21784-21794 (2015).
- Ľ. Jankovič, J. Kronek, J. Madejová, V. Hronský. (9,10-dihydroxyoctadecyl)ammonium: a structurally unique class of clay intercalable surfactants. European Journal of Inorganic Chemistry 17, 2841-2850 (2015).

Projects

- Photoactive hybrid nanomaterials with luminescent and antimicrobial properties. APVV-0291-11, 2012-2015
- Hybrid materials based on layered silicates with cyanine and porphyrine dyes. Vega 2/0107/13, 2013-2016

1. Research highlights – Department of Theoretical Chemistry

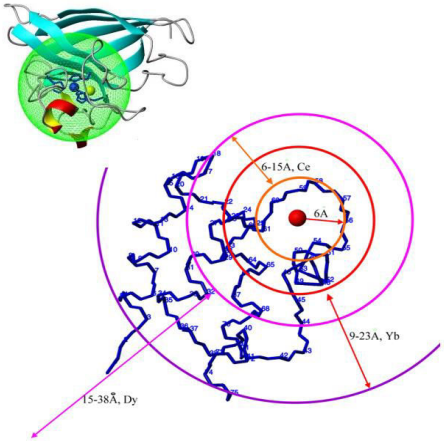
Fields of interest:

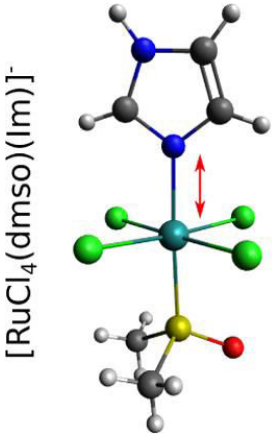
- development of advanced computational methods for electron correlation in molecules and solids
- development of relativistic methods for calculation of NMR and EPR parameters and application to heavy elements containing compounds
- development of methods for interpretation and visualization of spectroscopic properties
- molecular spectroscopy simulations by solution of time-dependent Dirac equation
- X-ray and neutron diffraction structural analysis supported by DFT solid state calculations
- application of quantum-chemical methods to wide class of chemical problems

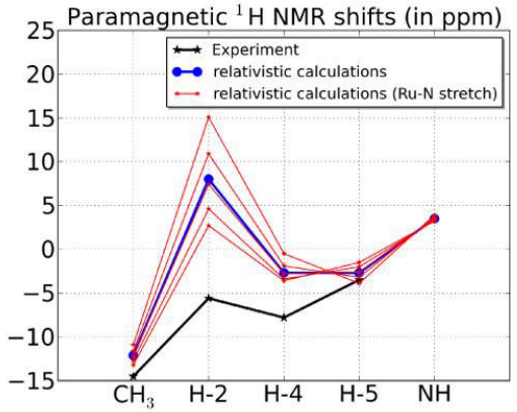
Theoretical approach for prediction and interpretation of pNMR spectra

Projects

FP7-Marie Curie Initial Training Networks: Pushing the envelope of nuclear magnetic resonance spectroscopy for paramagnetic systems. A combined experimental a theoretical approach (pNMR), (2013-2016)





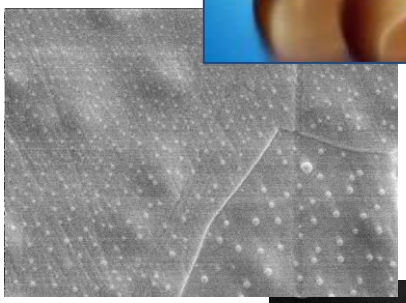


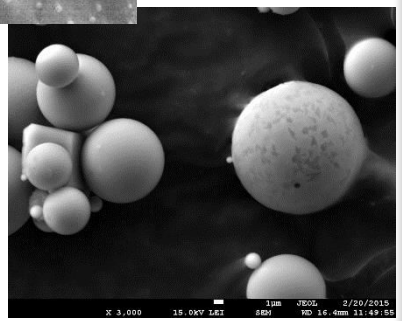
Publications

- S. Komorovský, M. Repiský, K. Ruud, O. L. Malkina, and V. G. Malkin, Four-Component Relativistic Density Functional Theory Calculations of NMR Shielding Tensors for Paramagnetic Systems. J. Phys. Chem. A, 117, 9235-9244 (2013) .
- S. Komorovský, M. Repiský, K. Ruud, O. Malkina, V. Malkin, Four-component relativistic density functional theory calculations of NMR shielding tensors for paramagnetic systems. J. Phys. Chem. A, 117, 14209-14219 (2013).
- M. Bühl, F.R. Knight, A. Křístková, I. Malkin-Ondík, O. Malkina, R.A.M. Randall, A.M.Z. Slawin, J.D. Woolins, Weak Te, Te interactions through the looking glass of NMR spin-spin coupling. Angewandte Chemie - International Edition, 52, 2495-2498 (2013).

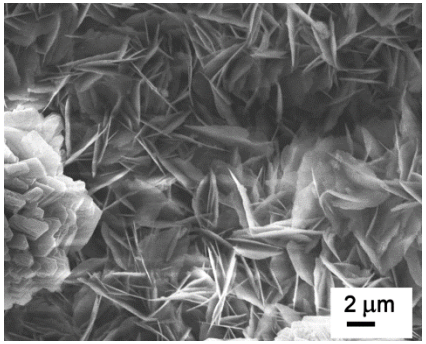
1. Research highlights – Joint Glass Centre of the IIC SAS, TnUAD and FChFT STU

Fields of interest:





- Oxide ceramic materials and ceramic matrix composites
- Corrosion of ceramic and glass materials, including biomaterials
- Composition, structure and properties of oxide, especially silicate glasses with industrial potential
- Glasses with additional functionalities (e.g. luminescence)



1. Research highlights – Joint Glass Centre of the IIC SAS, TnUAD and FChFT STU

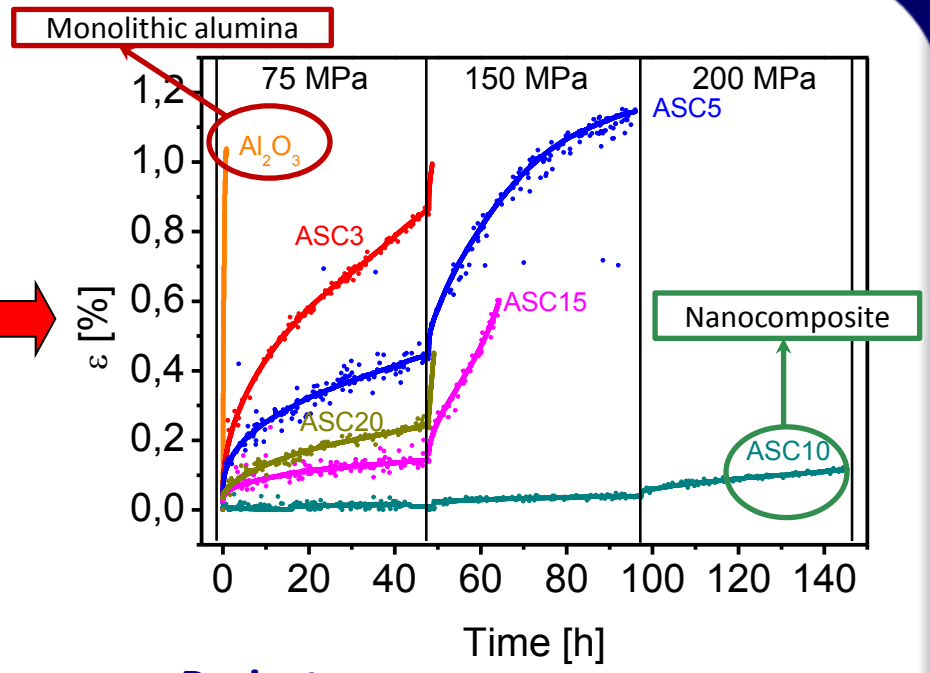
Alumina-based (nano)composites with enhanced properties

Alumina-based nanocomposites:

- SiC nanoparticles
- MWCNT

Enhanced properties:

- Wear resistance
- High temperature creep resistance
- Enhanced electric conductivity



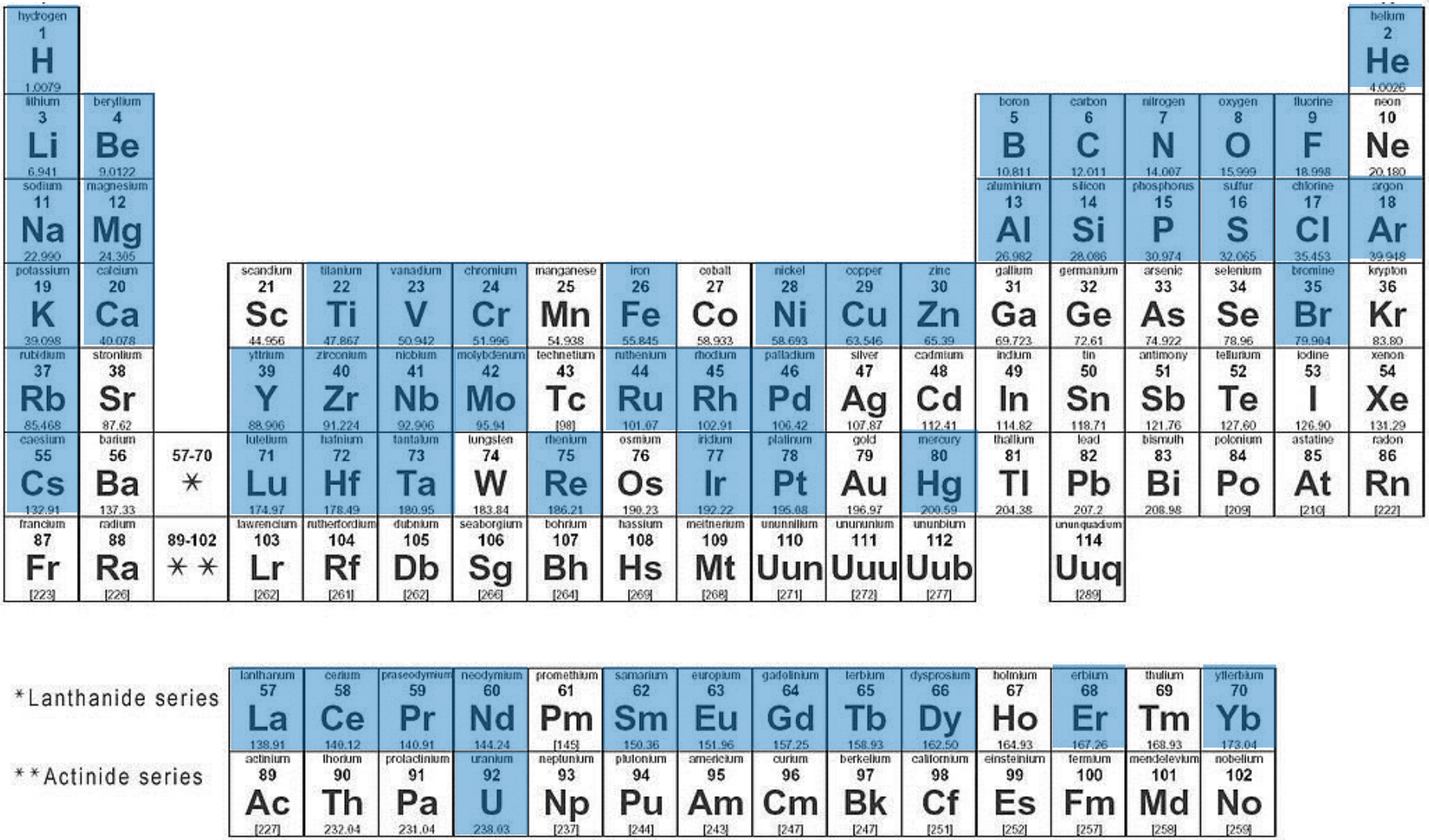
Publications

- M. Michálek, J. Sedláček, M. Parchovianský, M. Michálková, D. Galusek, Mechanical properties and electrical conductivity of alumina/MWCNT and alumina/zirconia/MWCNT composites, *Ceram. Int.* 40, 1289-1295 (2014).
- M. Michálek, M. Kašiarová, M. Michálková, D. Galusek, Mechanical and functional properties of Al_2O_3-ZrO_2-MWCNT nanocomposites, *J. Eur. Ceram.Soc.*34, 3329-3337 (2014).
- M. Parchovianský, D. Galusek, M. Michálek, P. Švančárek, M. Kašiarová, J. Dusza, M. Hnatko, Effect of the volume fraction of SiC on the microstructure, and creep behavior of hot pressed Al_2O_3/SiC composites, *Ceram. Int.* 40, 1807–1814 (2014).

Projects

- **NATO SfP 97 41 22**
  Alumina-Based Nano/Microcomposite Cutting Tools for High Speed Metal Cutting
- **LPP 0297-09**
  Ceramic composite with percolated phase prepared by infiltration with organometallic precursors
- **VEGA 2/3101/23**
  Ceramic alumina-based nanomaterials

1. Research highlights



2.1. Scientific output - publications

IF	Number of publications (ADC and ADD)			
	2012	2013	2014	2015
< 1	10	9	5	6
1-2	18	29	12	9
2-3	11	8	24	25
3 and more	13	12	8	7
	52	58	49	47

Year	2012	2013	2014	2015
Average IF	2.329	2.517	2.255	2.396
Median IF	1.751	1.789	2.086	2.353
Ratio of Q1 and Q2	60-70% Q1+Q2	52-72% Q1+Q2	71-80% Q1+Q2	56-80% Q1+Q2

2.2. Feedback on scientific outputs - responses

	2012	2013	2014	2015
WOS + Scopus	1234	1427	1445	1381

J. Noga	**1176**	**Department of Theoretical Chemistry**
J. Madejová	**1137**	**Department of Hydrosilicates**
P. Komadel	**907**	**Department of Hydrosilicates**
V. Malkin	**848**	**Department of Theoretical Chemistry**
O. Malkina	**791**	**Department of Theoretical Chemistry**
J. Bujdák	**628**	**Department of Hydrosilicates**
P. Šajgalík	**411**	**Department of Ceramic**

H-index of the Institute considering publications published within 2012-2015 stands at 17

2.3. Scientific status of the Institute in the international and domestic context

Participation in international multilateral projects

- **FP-7 - 2x**
- **COST – 2x**
- **ERANET – 1x**
- **Horizon 2020:**
  - Building-up Centre of Excellence for advanced materials application — CEMEA, 664337 - H2020-WIDESPREAD-2014-1; PC: Slovak Academy of Sciences; Partners: Finland - Teknologian tutkimuskeskus VTT OyEspo, HELSINGIN YLIOPISTO, Slovakia – 8 Institutes of SAS
  - **Centre for functional and surface-functionalized glasses, stage II – FunGlass, H2020-WIDESPREAD-2016-2017-739566; PC: TnUAD Slovakia; Partners: FAU Erlangen-Nuremberg, FSU Jena, Universita degli studi Padova, CSIC Madrid**

Submitted - not supported

- **MC - IF/ITN – 9/2**
- **H2020 - IA/RIA/ERC – 2/1/1**

International conferences (co)organised by the Institute – 10

Invited lectures of Institute employees at international conferences - 83

2.3. Scientific status of the Institute in the international and domestic context

INTERNATIONAL MOBILITY

Foreign guests at IIC SAS

Country	Number (persons)	Days spent at IIC
Argentina	1	10
Austria	2	199
China	1	41
Croatia	2	48
Czech Republic	10	149
France	2	8
Germany	2	84
India	2	119
Italy	1	4
Japan	1	14
Poland	3	238
Russia	3	74
Serbia	1	28
Sweden	2	65
USA	2	3
Overall	**35**	**1084**

IIC SAS researchers abroad

Country	Number (persons)	Days spent at partner
Austria	2	21
Belgium	3	100
China	2	41
Czech Republic	34	218
France	15	122
Germany	16	606
Great Britain	3	18
Hungary	1	5
Italy	3	14
Japan	4	149
Norway	2	41
Poland	6	99
Russia	5	127
South Korea	1	5
Sweden	2	67
Switzerland	1	7
Taiwan	2	19
Turkey	4	12
USA	1	6
Ukraine	2	16
Overall	**48**	**1715**

2.3. Scientific status of the Institute in the international and domestic context

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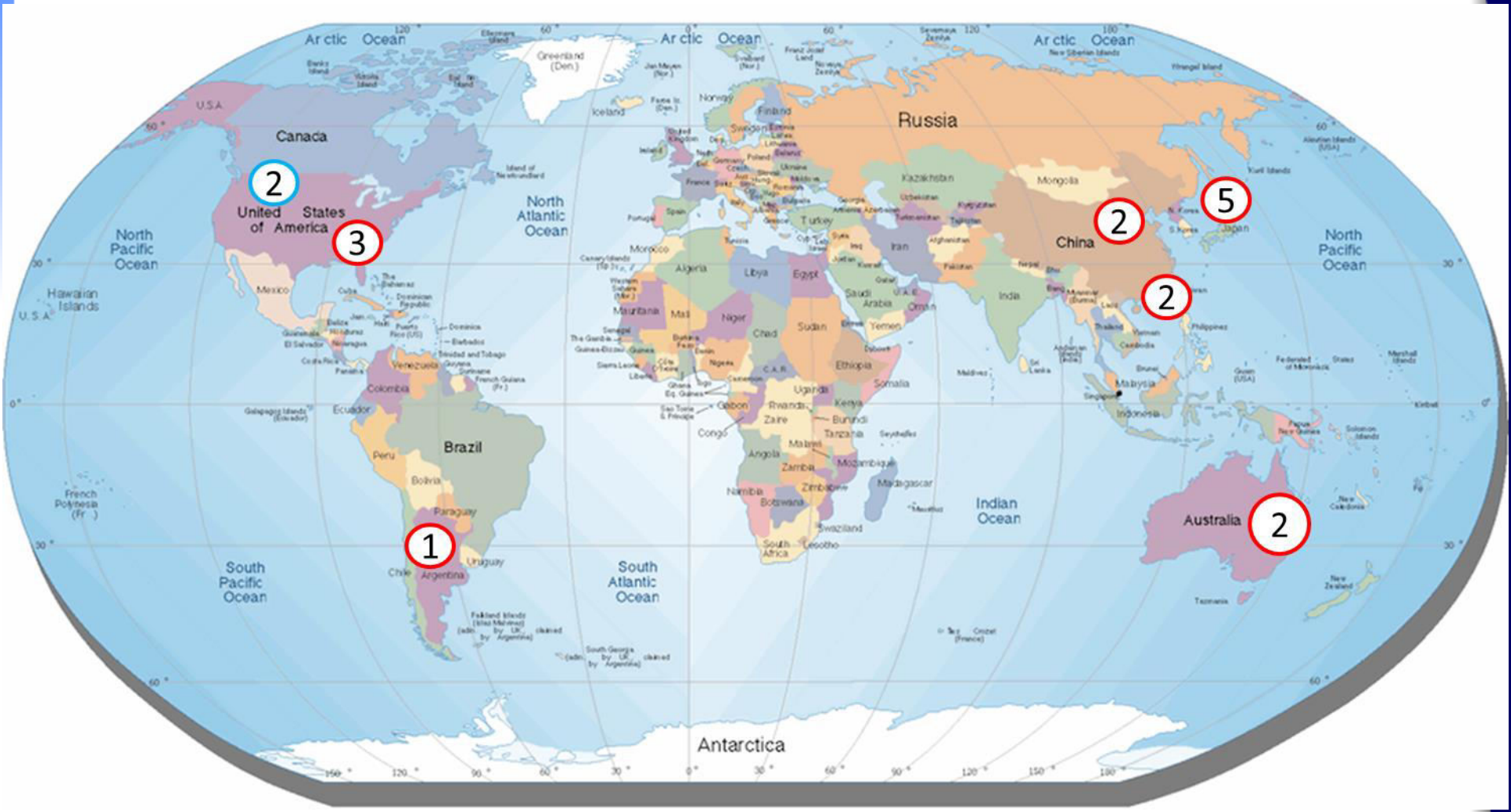


2.4. Projects

- **Projects of the Slovak Research and Development Agency (APVV)**

  Projects coordinated by IIC - 7

  Projects sub-coordinated by IIC – 3

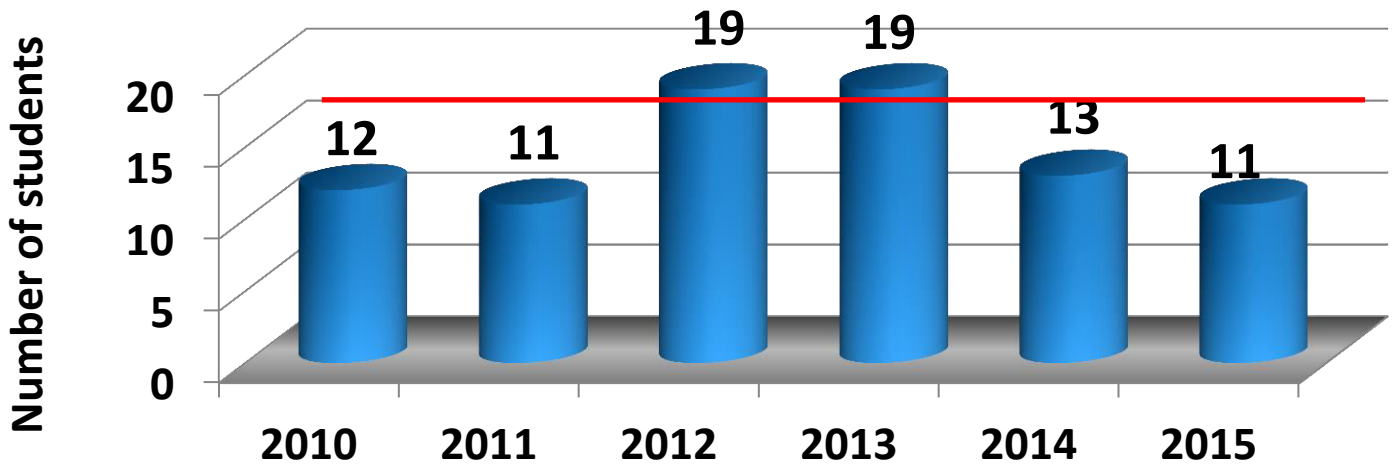
  Bilateral projects – 5

  Starting in 2016 - 6 + 2

- **Projects of the Scientific Grant Agency of the Slovak Academy of Sciences and the Ministry of Education (VEGA)** – 20
- **Projects of SAS Centres of Excellence** – 1
- **International projects supported from sources of SAS (MVTS)** - 9
- **National projects supported by EU Structural Funds** – 13
- **Projects supported from other sources**

2.5. Postgraduate studies and other educational activities

internal + external PhD students



		2010	2011	2012	2013	2014	2015
Foreign students	A			1	1	1	1
	CZ	1	1	4	4	2	
	Egypt				1	1	1
	UK				1	1	1
Defended PhD thesis		1	2	0	5	5	2

2.5. Postgraduate studies and other educational activities

Doctoral study fields:

Chemical Physics / 4.1.11

Faculty of Natural Sciences, Comenius University, Bratislava
Guarantor of the programme: prof. RNDr. Jozef Noga, DrSc.

Inorganic Chemistry / 4.1.15

Faculty of Natural Sciences, Comenius University, Bratislava
Guarantor of the programme: RNDr. Peter Komadel, DrSc.

Inorganic Technology and Materials / 5.2.19

Faculty of Chemical and Food Technology, Slovak University of Technology, Bratislava
Guarantor of the programme: prof. RNDr. Pavol Šajgalík, DrSc.

Competition of Young Researchers - annually organized in collaboration with the Institute of Inorganic Chemistry of the Academy of Sciences of the Czech Republic

2.6. Contribution to societal practice

Economic benefits

Patents

- Japanese - 3
- European – 1

Environmental benefits

- **Project oriented to magnesite processing and sewages processing**

"Study on the feasibility of Slovak magnesite processing by means of exploitation of extraction and processing sewages, and of magnesium-rich metal wastes, in line with innovative trends in the world, EU and Slovak Republic". 30/1020/2014-SPOL; Ministry of Education, Science, Research and Sport of the Slovak Republic.

- **Project oriented to utilizations of waste material produced by processing of perlite**

"Perlite genesis and innovative approaches to its exploitation and processing", APVV-0339-2012, 2013-2017, coordinator: Faculty of Natural Sciences CU, Bratislava

Social benefits

- Decrease unemployment - wide spectrum of positions

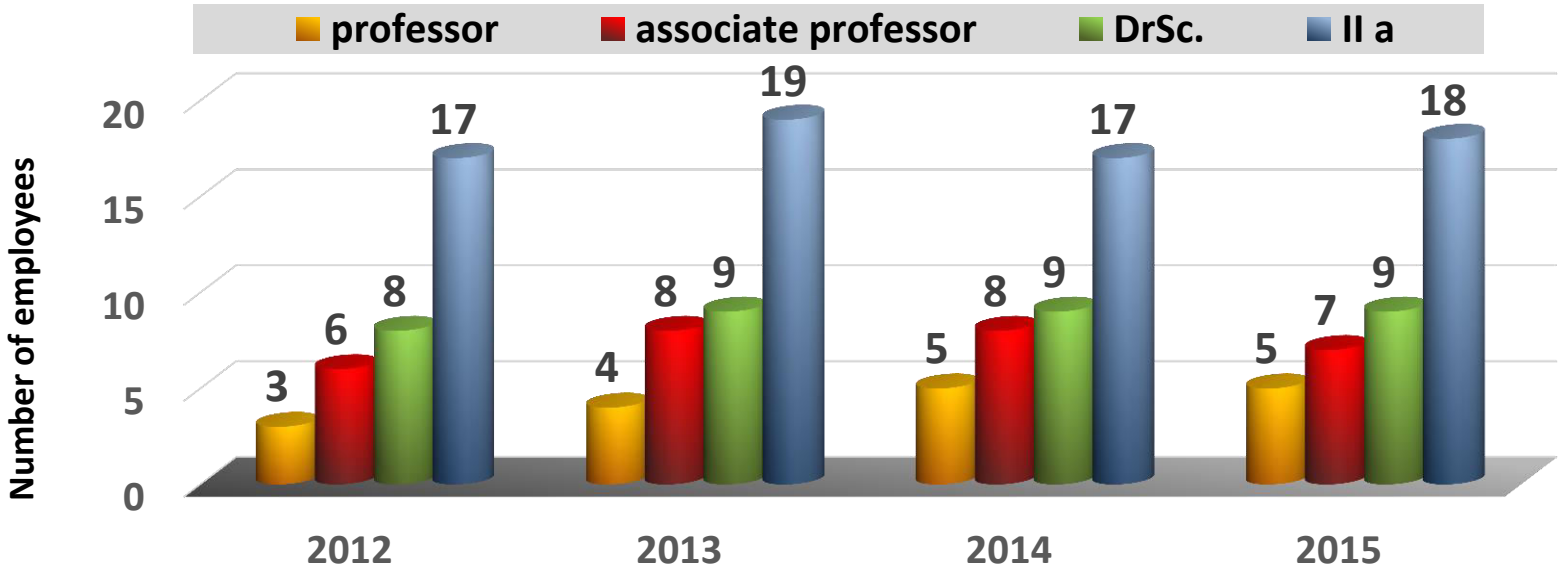
Cultural benefits

Research on archaeological artefacts or paintings

2.7. Popularization activities

- The Open Door Day – ca **200 visitors** annually
- The European Researchers' night – annual participation
- Articles in printed media, TV appearances and interviews broadcasted on radio
- The corresponding seminars in chemistry, biology and natural sciences for – **9 600 students of primary schools** and **930 students of secondary schools** (school years 2011/2012 and 2012/2013);
- Chemistry Olympiads - participation of the Institute members in national committees
- Public popularisation lectures – Super-school of Petržalka (primary schools), Scientific Super-school (primary schools), Comenius University for Children (primary schools), Workshops on chemistry, biology and natural sciences (primary and secondary schools)

2.8. Personnel development



- **SAS stipends and SASPRO stipends**
  HITEMPCORR - High-temperature properties of materials corrosion in molten salts**, 11/2015** - 11/2016, No: 1119/02/02, coordinator IIC: M. Boča, aplicant: Dr. Niketan Sarabhai Patel, India
- **Internal funding - the Slovak Academy of Sciences Supporting Fund of Stefan Schwarz**
  Mgr. Stanislav Kedžuch, PhD. (2008 - 2012)
- **Within Program for Human Potential Support in R&D and Science Popularization - 2**

Conclusion: personal structure is balanced both in age and in professional qualification

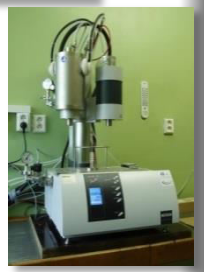
2.8. Infrastructure

- **Phase, microstructural and chemical analysis**

  SEM, XRD powder diffractometers,
  C/S analyzer, O/N/H analyzer, …


- **Determination of physico-chemical and mechanical properties of materials**

  TG/DTA/DSC analyzer with IR and MS,
  thermomechanical analyzer, rheometer, zeta
  potential analyzer, …

- **Spectral methods**

  XRF spectrometer, FTIR spectrometer,
  fluorescence spectrophotometer,
  UV-VIS spectrophotometer, Raman spectrometer, ...


- **Preparation and machining of ceramic and glass samples**

  Hot press elatec control, hot isostatic press,
  optical profile grinding machine, abrasive
  cutter, plasma system FEMTO, ...


- **Preparation and machining of other samples**

  Glove box, planetary mill, vibratory micro mill,
  freeze dryer, ...


3. Research strategy and future development

The mission of the Institute

- basic research of inorganic and bioinorganic systems aimed at the optimization and development of new materials and technologies
- upbringing (education) of new scientists in relevant areas
- contribution to the research and development in joint fields of interest in Slovak Republic and abroad by expertise and collaboration with universities and industrial partners

Define targets/aims/objectives – realistic and feasible

The vision of the Institute

- dignified and respectable research partner
- participate in the further development of scientific fields which the Institute was established for and has accumulated significant experience in
- part of the inter/multi/disciplinary scientific community

3. Research strategy and future development

Pillars *vs.* tools

Human sources

- looking for students and postdocs from abroad (at least one each year in average): H2020 – MC, ERC; Euraxess; Memorandum on student exchange with China, Korea, (India)
- to intensify mobility of researchers with stress to young researchers (each PhD student is obliged to spent at least three months abroad)
- to train young researcher – to become candidates for ERC, team leaders, members of executive body and scientific board – to avoid generation gap
- to train high level experts for existing infrastructure
- increase the number of senior researchers (from 28 at present to 35)

3. Research strategy and future development

Cooperation

- exploitation of pan-European infrastructure like synchrotron sources, XFEL… (to apply at least for two projects each year)
- to increase involvement in the research with industrial partners
- to increase bilateral exchange (at least two middle term stays per year)
- to create the communication centre between researchers and industry

Infrastructure

- to sustain existing one
- to increase effectiveness of operation and to extend optionality
- to extend with new methods

Financial sources

- to increase participation in large international projects (successful application of H2020 projects – at least two);
- increase the ratio of industrial support (to double actual state)

3. Research strategy and future development

Research areas of a primary focus:

- Materials for energy applications
- New technologies
- Domestic raw materials
- Biomaterials / materials for health care
- Other functional materials

Strategic documents

- Research and Innovation Strategy for Smart Specialisation (RIS3) SK
- Strategic Energy Technology (SET) Plan – European commission

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

Thank you for attention