

Ústav anorganickej chémie SAV



Správa o činnosti organizácie SAV za rok 2017

Bratislava
január 2018

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1. Základné údaje o organizácii

1.1. Kontaktné údaje

Názov: Ústav anorganickej chémie SAV

Riaditeľ: doc. Ing. Miroslav Boča, DrSc.

Zástupca riaditeľa: doc. Ing. Miroslav Hnatko, PhD.

Vedecký tajomník: doc. Ing. Zoltán Lenčéš, PhD.

Predseda vedeckej rady: RNDr. Jana Madejová, DrSc.

Člen snemu SAV: doc. Ing. Miroslav Hnatko, PhD.

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Názvy a adresy detašovaných pracovísk:

- **Vitrum Laugaricio - Centrum kompetencie skla, spoločné pracovisko ÚACH SAV, TnU AD, RONA, a.s. a FCHPT STU**
Študentská 2, 911 50 Trenčín
- **VC SAV – Pavilón materiálových vied**
Dúbravská cesta 9/6319, Bratislava
- **Pracovisko pre röntgenovú práškovú difraktometriu**
Ústav merania SAV, Dúbravská cesta 9, 841 04, Bratislava 4

Vedúci detašovaných pracovísk:

- **Vitrum Laugaricio - Centrum kompetencie skla, spoločné pracovisko ÚACH SAV, TnU AD, RONA, a.s. a FCHPT STU**
prof. Ing. Dušan Galusek, DrSc.
- **VC SAV – Pavilón materiálových vied**
doc. Ing. Miroslav Boča, DrSc.
- **Pracovisko pre röntgenovú práškovú difraktometriu**
doc. Ing. Miroslav Boča, DrSc.

Typ organizácie: Rozpočtová od roku 1953

1.2. Údaje o zamestnancoch

Tabuľka 1a Počet a štruktúra zamestnancov

Štruktúra zamestnancov	K	K		K do 35 rokov		F	P	T
		M	Ž	M	Ž			
Celkový počet zamestnancov	72	38	34	8	7	67	60,17	44,34
Vedeckí pracovníci	46	31	15	7	3	44	39,09	39,09
Odborní pracovníci VŠ (výskumní a vývojoví zamestnanci ¹)	6	2	4	1	2	4	4,25	4,25
Odborní pracovníci VŠ (ostatní zamestnanci ²)	6	3	3	0	2	6	4,88	1
Odborní pracovníci ÚS	12	2	10	0	0	11	9,95	0

Ostatní pracovníci	2	0	2	0	0	2	2	0
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¹ odmeňovaní podľa 553/2003 Z.z., príloha č. 5

² odmeňovaní podľa 553/2003 Z.z., príloha č. 3 a č. 4

K – kmeňový stav zamestnancov v pracovnom pomere k 31.12.2017 (uvádzať zamestnancov v pracovnom pomere, vrátane riadnej materskej dovolenky, zamestnancov pôsobiacich v zahraničí, v štátnych funkciách, členov Predsedníctva SAV, zamestnancov pôsobiacich v zastupiteľských zboroch)

F – fyzický stav zamestnancov k 31.12.2017 (bez riadnej materskej dovolenky, zamestnancov pôsobiacich v zahraničí v štátnych funkciách, členov Predsedníctva SAV, zamestnancov pôsobiacich v zastupiteľských zboroch)

P – celoročný priemerný prepočítaný počet zamestnancov

T – celoročný priemerný prepočítaný počet riešiteľov projektov

M, Ž – muži, ženy

Tabuľka 1b Štruktúra vedeckých pracovníkov (kmeňový stav k 31.12.2017)

Rodová skladba	Pracovníci s hodnosťou				Vedeckí pracovníci v stupňoch		
	DrSc.	CSc./PhD.	prof.	doc.	I.	II.a.	II.b.
Muži	8	22	4	6	8	14	9
Ženy	2	13	0	0	2	6	7

Tabuľka 1c Štruktúra pracovníkov podľa veku a rodu, ktorí sú riešiteľmi projektov

Veková štruktúra (roky)	< 31	31-35	36-40	41-45	46-50	51-55	56-60	61-65	> 65
Muži	3	6	5	8	2	2	1	6	1
Ženy	1	1	3	3	3	1	1	2	0

Tabuľka 1d Priemerný vek zamestnancov organizácie k 31.12.2017

	Kmeňoví zamestnanci		Vedeckí pracovníci		Riešitelia projektov	
	A	B	A	B	A	B
Muži	46,7	45,2	44,7	43,5	44,6	43,5
Ženy	47,0	47,2	43,1	43,3	45,7	46,0
Spolu	46,8	46,2	44,2	43,4	44,9	44,3

A - Prepočet bez zohľadnenia úväzkov zamestnancov

B - Prepočet so zohľadnením úväzkov zamestnancov

1.3. Iné dôležité informácie k základným údajom o organizácii a zmeny za posledné obdobie (v zameraní, v organizačnej štruktúre a pod.)

Ústav anorganickej chémie SAV v roku 2017 nezaznamenal žiadne zásadné zmeny v organizačnej štruktúre.

Priemerný vek zamestnancov ÚACH SAV dlhodobo ostáva pod hranicou 47 rokov. V roku 2017 bol priemerný vek všetkých pracovníkov ústavu 46,8 roka a priemerný vek vedeckých pracovníkov 44,2. Napriek tomu, že zamestnávanie mladých schopných post-doktorandov na ústave je jednou z hlavných priorít, nevieme ju v požadovanej miere primerane naplniť. Ak sa podarí nejakého mladého vedeckého pracovníka po skončení PhD štúdia zamestnať, tak len cez projekty, a to znamená, že na dobu 2-3 rokov, za tabuľkovú mzdu. Mnohí z mladých vedeckých pracovníkov takúto ponuku odmietnu. Z toho plynie aj pravdepodobné zvyšovanie priemerného veku zamestnancov v blízkej budúcnosti, keďže počet pracovníkov v dôchodkovom veku je minimálny a prirodzená generačná výmena je obmedzená. Takáto situácia kladie nároky na personálnu a predovšetkým mzdovú politiku vedenia ústavu. Motivácia mladých pracovníkov pre zotrvanie na ústave sa realizuje predovšetkým prostredníctvom poskytnutia možnosti zvyšovania ich kvalifikácie (stupeň IIb, IIa a Ia). Zvyšovanie kvalifikácie vedeckých pracovníkov má logicky za následok zvýšený tlak na mzdový fond. Tento fakt by mohlo pri tvorbe rozpočtu, hlavne mzdových fondov ústavov, zohľadniť aj vedenie SAV pri presadzovaní vlastnej mzdovej politiky v rámci SAV. Ústav sa od roku 2008

podieľal na realizácii 13-tich projektov financovaných zo ŠF EÚ, ktoré sú aktuálne všetky ukončené. Aj napriek tomu, že tieto projekty sú ukončené, administratívne zaťaženie na ich monitoring ostáva, pričom mzdové náklady na túto administráciu už nie je možné vykrývať z projektov, ale len zo mzdového fondu. Navyše, výraznú časť administratívnych výkonov preberajú aj vedeckí pracovníci. Prepočítaný počet pracovníkov v roku 2017 je na úrovni 60,19 FTE, čo je porovnateľný stav s rokom 2016 (59,43). Treba tiež upozorniť, že do tohto počtu vstupujú aj traja štipendisti programu SASPRO a zamestnanci platení z projektov APVV.

2. Vedecká činnosť

2.1. Domáce projekty

Tabuľka 2a Domáce projekty riešené v roku 2017

ŠTRUKTÚRA PROJEKTOV	Počet		Čerpané financie (€)					
	A	B	A				B	
			Zo zdrojov SAV		Z iných zdrojov		Zo zdrojov SAV	Z iných zdrojov
			Spolu	Pre organizáciu	Spolu	Pre organizáciu		
1. Projekty VEGA	9	1	103 549	103 549	-	-	4 051	-
2. Projekty APVV	7	4	-	-	410 655	286 816	-	59 433
3. Projekty OP ŠF	0	0	-	-	-	-	-	-
4. Projekty SASPRO	3	0	195 262	195 262	-	-	-	-
5. Projekty centier excelentnosti SAV	0	0	-	-	-	-	-	-
6. Iné projekty (FM EHP, ŠPVV, Vedecko-technické projekty, ESF, na objednávku rezortov a pod.)	0	0	-	-	-	-	-	-

A - organizácia je nositeľom projektu

B - organizácia sa zmluvne podieľa na riešení projektu

Tabuľka 2b Domáce projekty podané v roku 2017

Štruktúra projektov	Miesto podania	Organizácia je nositeľom projektu	Organizácia sa zmluvne podieľa na riešení projektu
1. Účasť na nových výzvach APVV r. 2017	-	5	2
2. Projekty výziev OP ŠF podané r. 2017	Bratislava		1
	Regióny		1

Projekty štrukturálnych fondov:

Názov projektu: Vybudovanie Centra pre využitie pokročilých materiálov Slovenskej akadémie vied

Evidenčné číslo projektu, výzva: Kód ŽoNFP: NFP313020K766, OPVaI-VA/DP/2017/2.1.1-03

Acronym: CEMEA

Podávateľ projektu: Slovenská akadémia vied

Partner/i: Centrum pre využitie pokročilých materiálov Slovenskej akadémie vied, Elektrotechnický ústav Slovenskej akadémie vied, University of Helsinki, Ústav anorganickej chémie SAV, Ústav polymérov Slovenskej akadémie vied

Stav: podaný

Názov projektu: Výskum progresívnych materiálov pre priemysel

Evidenčné číslo projektu: NFP313010C857

Acronym: PROGMAT

Podávateľ projektu: CEIT a.s.

Partner/i: Ústav anorganickej chémie SAV, Žilinská univerzita v Žiline

Stav: podaný, v zásobníku (prerušené hodnotenie podaných projektov)

Projekty APVV

Názov projektu: Vývoj žiaruvzdorných pyrochlórnych fáz pre vysokoteplotn aplikácie neoxidovej keramiky

Evidenčné číslo projektu: APVV-17-0328

Acronym: PyrMat

Podávateľ projektu: Ústav anorganickej chémie SAV (P. Tatarko)

Partner/i: ÚMV SAV Košice

Stav: podaný

Názov projektu: Nové sklené a sklokeramické fosfory na báze hlinitanov vzácnych zemín pre aplikácie v pevnolátkových energiách šetriacich svetelných zdrojoch vyžarujúcich biele svetlo (pc-WLED diódy).

Evidenčné číslo projektu: APVV-17-0049

Podávateľ projektu: WLEDMAT

Partner/i: ÚACH SAV, ÚMV SAV Košice

Stav: podaný

Názov projektu: Korózia a zvetrávanie úžitkových skiel

Evidenčné číslo projektu: APVV-17-0076

Acronym: KOROZ

Podávateľ projektu: Trenčianska univerzita Alexandra Dubčeka v Trenčíne

Partner/i: ÚACH SAV BA (D. Galusek), RONA, a.s.

Stav: podaný

Projekty APVV bilaterálne

Názov projektu: Rozpustnosť oxidov a plynov v roztavenom systéme KF-AlF₃

Evidenčné číslo projektu: SK-CN-2017-0020 (APVV)

Acronym: SOLOXIGAS

Podávateľ projektu: ÚACH SAV (B. Kubíková)

Partner/i: Northeastern University, Shenyang, Čína

Stav: podaný/zamietnutý

Názov projektu: Tepelná stabilita a štruktúrna korelácia rubídnych oxo- a oxo-fluóro-hlinitanov, ako tuhých iónových vodičov.

Evidenčné číslo projektu: SK-FR-2017-0010 (APVV)

Acronym: TISRAF

Podávateľ projektu: ÚACH SAV (F. Šimko)

Partner/i: Conditions Extrêmes et Matériaux: Haute Temperature et Irradiation (CEMHTI), CNRS, Orléans, France

Stav: podaný/zamietnutý

Názov projektu: Modelové štúdium interakcií hlinitokremičitanových nanorúrok s oxyaniónmi

Evidenčné číslo projektu: SK-AT-2017-0016 (APVV)

Acronym: HKNR-OA

Podávateľ projektu: ÚACH SAV (E. Scholtzová)

Partner/i: Institute for Soil Research of University of Natural Resources and Life Sciences, Viedeň, Rakúsko

Stav: podaný

Názov projektu: Spájanie moderných keramických materiálov na báze SiC / Joining of advanced SiC-based ceramic materials

Evidenčné číslo projektu: APVV, SK-CN-2017-0040,

Acronym: JOINSIC 2018-2019

Podávateľ projektu: Ústav anorganickej chémie SAV (P. Tatarko)

Partner/i: Speciality Fibers and Nuclear Energy Materials Engineering Laboratory, Ningbo Institute of Material Technology and Engineering (NIMTE), Chinese Academy of Sciences, Ningbo, People's Republic China

Stav: schválený

2.2. Medzinárodné projekty**2.2.1. Medzinárodné projekty riešené v roku 2017**

Tabuľka 2c Medzinárodné projekty riešené v roku 2017

ŠTRUKTÚRA PROJEKTOV	Počet		Čerpané financie (€)					
	A	B	A				B	
			Zo zdrojov SAV		Z iných zdrojov		Zo zdrojov SAV	Z iných zdrojov
			Spolu	Pre organizáciu	Spolu	Pre organizáciu		
1. Projekty 7. RP EÚ a Horizont 2020	1	0	-	-	-	-	-	-
2. Projekty ERA.NET, ESA, JRP	0	1	-	-	-	-	-	-
3. Projekty COST	0	2	-	-	-	-	-	-
4. Projekty EUREKA, NATO, UNESCO, CERN, IAEA, IVF, ERDF a iné	1	0	-	-	-	-	-	-
5. Projekty v rámci medzivládnych dohôd	1	0	-	-	-	-	-	-
6. Bilaterálne projekty MAD	1	0	-	-	-	-	-	-
7. Bilaterálne projekty ostatné	1	0	-	-	-	-	-	-
8. Podpora MVTs z národných zdrojov (SAV, APVV a iné)	4	3	28 998	28 998	5 215	5 215	12 275	-
9. Iné projekty	0	0	-	-	-	-	-	-

A - organizácia je nositeľom projektu

B - organizácia sa zmluvne podieľa na riešení projektu

2.2.2. Medzinárodné projekty Horizont 2020 podané v roku 2017

Tabuľka 2d Počet projektov Horizont 2020 v roku 2017

	A	B
Počet podaných projektov Horizont 2020	2	0

Názov projektu: Advanced nano-ceramics for green and environmental technologies

Evidenčné číslo projektu, výzva: Horizon 2020 MCSA-ITN-2017, SEP-210411931

Acronym: ADVANTAGES

Podávateľ projektu: ÚACH SAV (Z. Lenčoš)

Partner/i: Technische Universität Darmstadt – Nemecko, CNRS Montpellier – Francúzsko, CNRS Limoges – Francúzsko, Universität Bayreuth – Nemecko, Università degli Studi di Padova – Taliansko, Università degli Studi di Trento – Taliansko, EngiCer SA – Švajčiarsko, Saint-Gobain Centre de Recherches et D'Etudes Europeen – Francúzsko, Merck KGaA – Nemecko, Clemson University – USA, Nagoya Institute of Technology - Japonsko

Stav: neschválený

Názov projektu: New Generation Ultra-High Temperature Ceramic Matrix Composites for Aerospace Industry

Evidenčné číslo projektu: H2020-MSCA-IF-2017, Proposal number: 798651

Acronym: CeramCom

Podávateľ projektu: ÚACH SAV P. Tatarko

Partner/i: Central R&T, Airbus Defence and Space GmbH, Taufkirchen, Germany

Stav: podaný

A - organizácia je nositeľom projektu

B - organizácia sa zmluvne podieľa na riešení projektu

Údaje k domácim a medzinárodným projektom sú uvedené v Prílohe B.

2.2.3. Zámery na čerpanie štrukturálnych fondov EÚ v ďalších výzvach

Aj napriek aktuálnej politickej situácii okolo štrukturálnych fondov (ktorá je nedôstojná, nepochopiteľná a demotivujúca), ústav bude reagovať spolu so svojimi partnermi aj na ďalšie výzvy.

2.3. Najvýznamnejšie výsledky vedeckej práce (maximálne 1000 znakov + 1 obrázok; bibliografický údaj uvádzajte rovnako ako v zozname publikačnej činnosti, vrátane IF)

2.3.1. Základný výskum

Rezonančný prenos energie medzi molekulami farbiva v koloidoch vrstvených nanočastíc saponitu: Vplyv povrchovej koncentrácie farbiva.

Silvia Belušáková, Juraj Bujdák

Vysoko efektívny rezonančný prenos energie Försterovského typu (FRET) medzi molekulami farbív rodamínu 6G a oxazínu 4 sa pozoroval vo vodných koloidných systémoch s vrstevnatým kremičitanom, saponitom, už pri relatívne nízkych koncentráciách farbív. Vhodnou optimalizáciou sústav sa podarilo eliminovať molekulovú agregáciu, ktorá všeobecne vedie k zániku luminiscencie. Prenos energie primárne závisel na povrchovej koncentrácii molekúl farbív, ktorá sa menila vhodnou voľbou pomeru farbiva a saponitu. Výťažky prenosu energie boli stanovené metódami fluorescenčnej spektroskopie, najmä v časovo rozlíšenom móde. Hodnoty z nameraných spektier nezodpovedali vypočítaným priemerným medzimolekulovým vzdialenostiam z povrchovej koncentrácie farbív. Jedným z hlavných prínosov práce bolo vytvorenie modelu, ktorý dokázal pomerne presne predpovedať experimentálne získané výťažky FRET. Model uvažoval heterogénnu distribúciu molekúl a štatistickú pravdepodobnosť výskytu rôznych

vzdialeností medzi interagujúcimi molekulami. Informácie získané touto prácou môžu mať význam pre pochopenie zákonitostí a vlastností systémov hybridných koloidných sústav vrstevnatých nanočastíc s adsorbovanými molekulami farbív. Aplikácie takýchto systémov zahŕňajú optické a fotovoltaičné materiály, tuhé lasery, molekulové sondy, fotosenzibilizátory, fotokatalyzátory a fotodezinfekčné materiály.



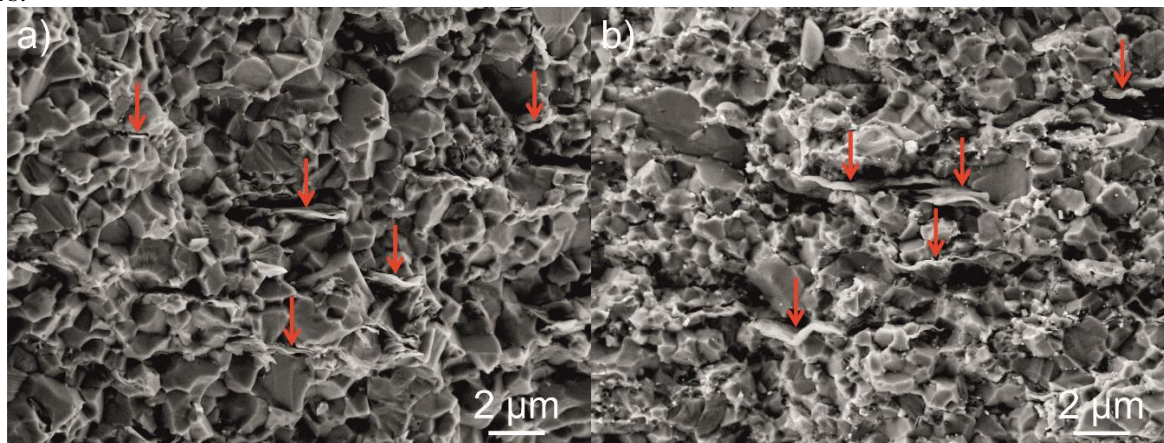
Obr: Zmena koncentrácie farbív na povrchu častíc saponitu a jej vplyv na fluorescenčné vlastnosti vznikajúcich hybridných sústav

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. Typ: ADCA

Uhlíkové nanočastice obsahujúce keramické kompozity s vysokou elektrickou vodivosťou

Ondrej Hanzel, Jaroslav Sedláček, Roman Bystrický, Valéria Bizovská, Pavol Šajgalík

V tejto práci boli novou metódou pripravené hutné kompozitné práškové zmesi na báze Al_2O_3 alebo SiC s prídavkom uhlíkových nanoštruktúr - uhlíkové nanorúrky (CNTs), grafénové nanoplatničky (GNPs). Tento proces zahŕňal funkcionizáciu uhlíkových nanoštruktúr, ich stabilizáciu v suspenzii a následné rozprašovanie takto stabilizovanej suspenzie do tekutého dusíka. Na týchto kompozitoch bol študovaný vplyv prídavku uhlíkových nanoštruktúr a vplyv orientácie na funkčné vlastnosti (elektrická a tepelná vodivosť). V prípade kompozitov Al_2O_3 -CNT sa podarilo významne zvýšiť elektrickú vodivosť (o 13 rádov) z hodnoty 10^{-10} S/m (čistý Al_2O_3) až na hodnotu 1748 S/m pre kompozit s prídavkom 12,5 obj. % CNTs. V prípade kompozitov SiC-GNPs sa podarilo zvýšiť elektrickú vodivosť (o 5 rádov) až na 1775 S/m. Toto zvýšenie elektrickej vodivosti možno pripísať metóde prípravy, ktorá umožňuje zachovať homogénnu distribúciu uhlíkových nanoštruktúr, ktoré v keramickej matici vytvárajú vodivú sieť. Výhodou keramických kompozitov so zvýšenou elektrickou vodivosťou je, že ich možno elektro-iskrovo obrábať. Efektívna obrábateľnosť týchto materiálov bola preukázaná pri kompozitoch s prídavkom $\geq 7,5$ obj. % CNTs.



Obr. Lomové plochy (a) SiC-GNPs a (b) SiC-GO kompozitov; šípky indikujú pozíciu grafénových štruktúr a smer pôsobenie tlaku počas spekania

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. (3.411 - IF2016). ISSN 0955-2219.

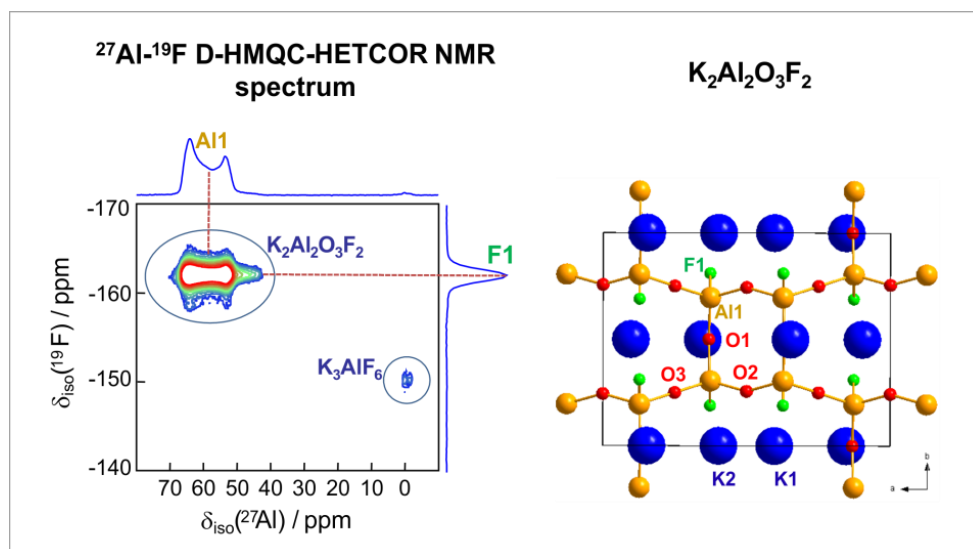
HANZEL, Ondrej - LOFAJ, František - SEDLÁČEK, Jaroslav - KABÁTOVÁ, Margita - KAŠIAROVÁ, Monika - ŠAJGALÍK, Pavol. Mechanical and tribological properties of alumina-MWCNTs composites sintered by rapid hot-pressing. In Journal of the European Ceramic Society, 2017, vol. 37, no. 15, p. 4821-4831. (3.411 - IF2016). ISSN 0955-2219.

SINGH, Meinam Annebushan - SARMA, Deba Kumar - HANZEL, Ondrej - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Machinability analysis of multi walled carbon nanotubes filled alumina composites in wire electrical discharge machining process. In Journal of the European Ceramic Society, 2017, vol. 37, no. 9, p. 3107-3114. (3.411 - IF2016). ISSN 0955-2219.

Tepelná stabilita a štruktúrna korelácia oxo- a oxo-fluóro-hlinitanov draselných v systéme KF-Al₂O₃.

Šimko František, Rakhmatullin Aydar, Florian Pierre, Kontrík Martin, Korenko Michal, Netriová Zuzana, Danielik Vladimír, and Bessada Catherine

Uskutočnila sa komplexná štruktúrna a fázová analýza systému KF-Al₂O₃ (1). Metódou termickej analýzy sa zadefinovali fázové polia vo fázovom diagrame a identifikovali sa tuhé fázy, existujúce v skúmanom systéme. Systém reprezentuje stabilnú diagonálu kvartérneho systému KF-Al₂O₃-AlF₃-K₂O. Analýzy fázových polí ukázali prítomnosť veľkého množstva komplexných zložiek v systéme, a to K₃AlF₆, KAlF₄, KAlO₂, KAl₉O₁₄, KAl₁₁O₁₇ a K₂Al₂O₃F₂. Všetky uvedené zlúčeniny boli tiež pripravené v čistom stave. Vykonala sa ich štruktúrna charakterizácia v tuhom stave s použitím najnovších NMR techník, vrátane MQ-MAS a D-HMQC, ktoré poskytli nový a jasnejší pohľad na ich vzájomnú štruktúrnú koreláciu. Išlo o štruktúrnú podobnosť kovalentne viazaných FO₂Al-O-AlO₂F tetraédrov v štruktúre K₂Al₂O₃F₂ s usporiadaním O₃Al-O-AlO₃ tetraédrov v štruktúre oxohlinitanu "mullitového" typu, KAl₁₁O₁₇. Z analýzy jednotlivých fázových polí vyplýva aj vzájomné metastabilné správanie objavených zložiek v systéme.



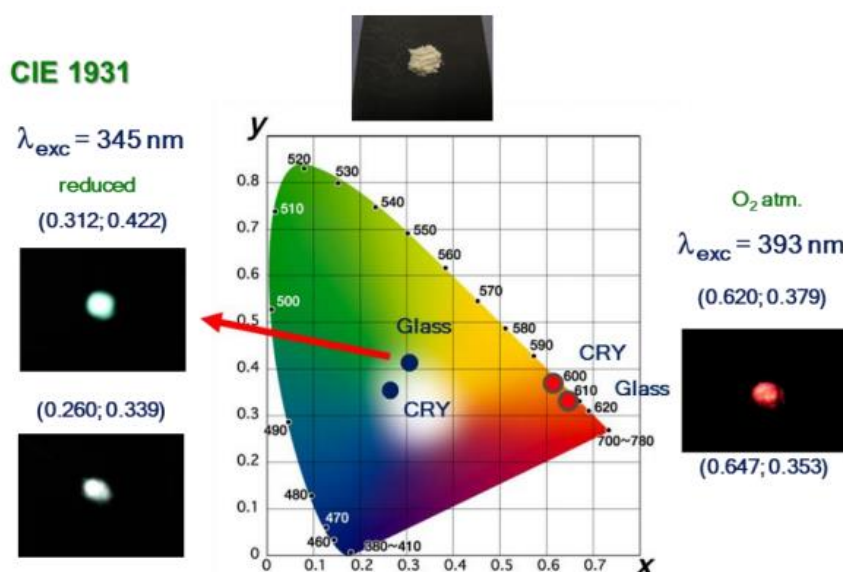
Obr: Separácia ²⁷Al a ¹⁹F NMR signálu čistého K₂Al₂O₃F₂ pomocou ²⁷Al-¹⁹F D-HMQC HETCOR MAS NMR analýzy na vzorke zloženia 2KF/1Al₂O₃.

ŠIMKO, František - 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. (4.857 - IF2016). ISSN 0020-1669. Typ: ADCA

Nové anorganické fosfory na báze hlinitanov vzácnych zemín pre aplikácie v LED diódach vyžarujúcich biele svetlo

Robert Klement, Katarína Haladejová, Anna Prnová, Jana Valúchová, Dušan Galusek, Katarína Drdlíková, Jozef Kraxner, Peter Švančárek, Milan Parchovianský

Pripravené boli sklo-polykryštalické fosfory v sústavách $\text{Y}_2\text{O}_3\text{-Al}_2\text{O}_3$ a $\text{Y}_2\text{O}_3\text{-Al}_2\text{O}_3\text{-SiO}_2$ dopované iónmi $\text{Ce}^{3+}\text{-Mn}^{2+}/\text{Mn}^{4+}$ a $\text{Eu}^{2+}/\text{Eu}^{3+}$ vyžarujúce biele svetlo, so zvýšenou emisiou v červenej spektrálnej oblasti, po excitácii NUV žiarením. Ióny Ce^{3+} zabudované v YAG matici vykazujú žltu-zelenú emisiu, zatiaľ čo ióny vo zvyškovej sklenej fáze modrú emisiu pri excitácii NUV žiarením. Tým možno riadenou kryštalizáciou pripraviť systém emitujúci biele svetlo. Veľmi sľubné výsledky poskytuje systém $\text{Y}_2\text{O}_3\text{-Al}_2\text{O}_3$ dopovaný $\text{Eu}^{2+}/\text{Eu}^{3+}$ iónmi (Obr.). Vzhľadom na prítomnosť oboch oxidačných stavov Eu v matici (Eu^{2+} intenzívne emituje v oblasti 400-700 nm, Eu^{3+} typický emitér červeného svetla) možno dosiahnuť emisiu bieleho svetla, pričom ladením vlnovej dĺžky excitujúceho žiarenia je možné efektívne zvýšiť podiel emisie červeného svetla vo výslednom bielom svetle. Nespornou výhodou je najmä využitie len jedného RE iónu v pomerne nízkej koncentrácii v matici, na rozdiel od známych fosforov kde je na emisiu bieleho svetla nevyhnutná prítomnosť 2-3 rôznych RE iónov v jednej alebo viacerých fázach.



Obr.: CIE 1931 farebné súradnice svetla emitovaného vzorkou skla a polykryštalického materiálu v sústave $\text{Y}_2\text{O}_3\text{-Al}_2\text{O}_3$ s eutektickým zložením dopovanej $\text{Eu}^{2+}/\text{Eu}^{3+}$ iónmi po excitácii NUV žiarením. Fotografie reprezentujú redukované alebo oxidované vzorky ožiarené UV svetlom pri 345 a 393 nm.

PRNOVÁ, A. - KLEMENT, R. - BODIŠOVÁ, K. - VALÚCHOVÁ, J. - GALUSEK, D. - BRUNEEL, E. - VAN DRIESSE, I. Thermal behaviour of yttrium aluminate glasses studied by DSC, high-temperature X-ray diffraction, SEM and SEM-EDS, *Journal of Thermal Analysis and Calorimetry* 128 (2017) 1407-1415. IF=1.953

PRNOVÁ, A. - PLŠKO, A. - VALÚCHOVÁ, J. - HALADEJOVÁ, K. - KLEMENT, R. - GALUSEK, D. Crystallization kinetics of glass microspheres with yttrium aluminium garnet (YAG) composition, *Journal of Thermal Analysis and Calorimetry*, (2017) in press, DOI: 10.1007/s10973-017-6690-9.

DRDLÍKOVÁ, K. - KLEMENT, R. - HADRABA, H. - DRDLÍK, D. - GALUSEK, D. - MACA, K. Luminescent Eu^{3+} -doped transparent alumina ceramics with high hardness, *Journal of European Ceramics Society* 37 (2017) 4271-4277. IF: 3.411

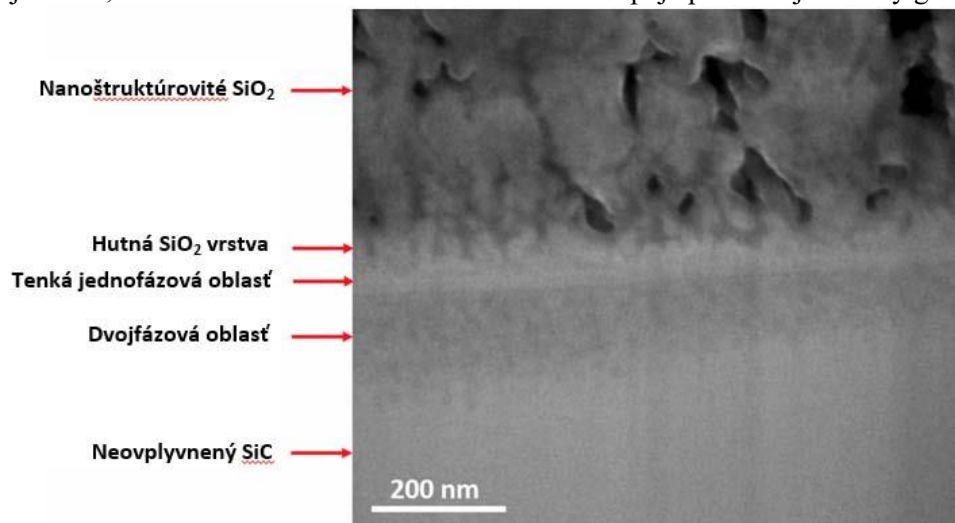
DRDLÍKOVÁ, K. - KLEMENT, R. - DRDLÍK, D. - SPUSTA, T. - GALUSEK, D. - MACA, K. Luminescent Er^{3+} -doped transparent alumina ceramics, *Journal of European Ceramics Society* 37 (2017) 2695-2703. IF: 3.411

2.3.2. Aplikačný typ

Vplyv pulznej laserovej radiácie na povrch SiC

Peter Tatarko, Pavol Šajgalík

V tejto práci bol študovaný vplyv laserového opracovania povrchu monolitného Boostec® SiC na mechanizmus spájania a vlastnosti spojov s epoxidovým lepidlom Hysol®. Tento výskum nadviazal na predchádzajúce aktivity realizované firmou Airbus Group Innovations and Airbus DS GmbH, ktoré jednoznačne preukázali, že laserová radiácia predstavuje veľmi efektívnu novú technológiu pre predúpravu povrchu kovov a keramiky Si_3N_4 . Laserom modifikovaná povrchová vrstva SiC (realizované firmou Airbus Group) bola detailne študovaná z hľadiska mikroštruktúry a chemického zloženia pomocou FIB SEM a HRTEM, AFM, XPS, EDX, and microXRD. Na základe výsledkov bol po prvýkrát detailne popísaný mechanizmus tvorby laserom modifikovanej vrstvy SiC, pozostávajúcej z celkovo piatich zón. Na rozdiel od kovov a keramiky Si_3N_4 , laserová radiácia povrchu SiC na vzduchu viedla vždy k tvorbe grafitovej vrstvy v podpovrchovej oblasti, čím dochádzalo k oslabeniu a delaminácii spoja pozdĺž tejto vrstvy grafitu.



SEM snímka zobrazujúca pričný rez laserom ovplyvnenej povrchovej oblasti SiC. Tvorba grafitovej vrstvy v tenkej jednofázovej oblasti bola potvrdená pomocou HRTEM.

SUESS, Manuela - WILHELMI, Christian - SALVO, Milena - CASALEGNO, Valentina - TATARKO, Peter - FUNKE, Matthias. **Effect of pulsed laser irradiation on the SiC surface**. In International Journal of Applied Ceramic Technology, 2017, vol. 14, no. 3, p. 313-322. (1.048 - IF2016).ISSN 1744-7402

Práca vznikla v rámci riešenia medzinárodného **EU projektu** v programe **FP7 2007-2013** pod názvom „**ADMACOM**“ – Advanced manufacturing routes for metal/composite components for aerospace, č. 609188.

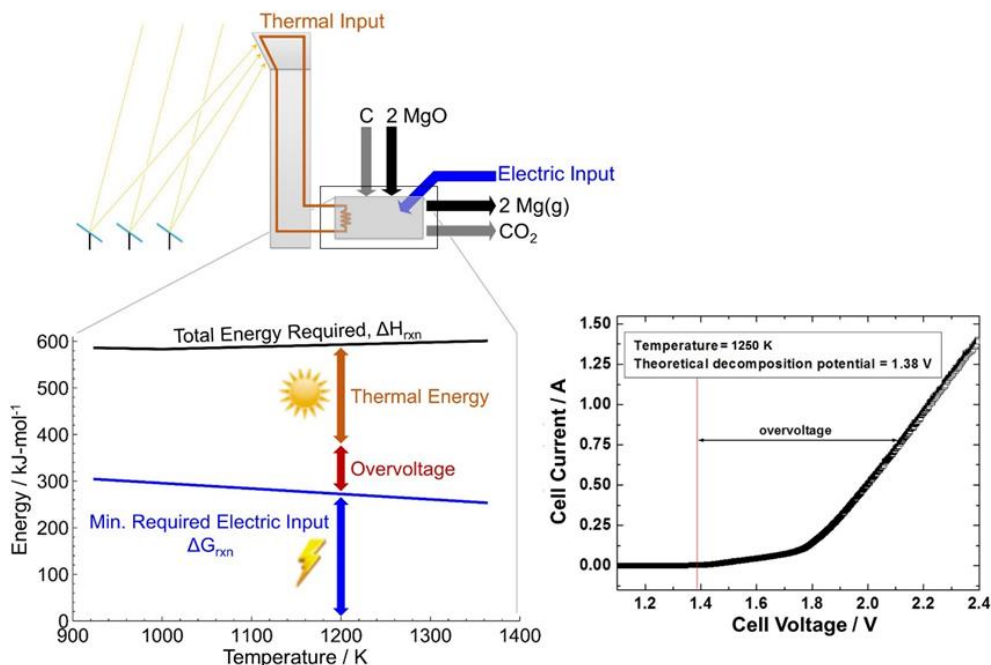
2.3.3. Medzinárodné vedecké projekty

Solárna tepelná elektrolyza horčička z roztavených fluoridov.

R. Palumbo, M. Korenko, N. Leonard, C. Larson, R. Diver, S. Nudehi, D. Blood, K. Blood, F. Šimko, L.J. Venstrom P. Kissinger

Projekt vývoja a technicko-ekonomickej analýzy novej ekologicko-ekonomickej výroby horčička za príspevku solárneho tepelného imputu. Pomocou analýzy prúdovej účinnosti sa vytypoval najvhodnejší fluoridový elektrolyt a zmerali sa základné termodynamické, transportné a kinetické charakteristiky procesu (vylučovacie potenciály, difúzne koeficienty, výmenné prúdové hustoty, elektrická vodivosť elektrolytu) tak, aby sa celý proces dal technicky a ekonomicky vyhodnotiť. Výsledkom procesu bol návrh úplne novej technológie výroby primárneho horčička, ktorý je ekologicky citlivý a zároveň ekonomicky konkurencie schopný hlavne vo vzťahu k dnes dominujúcemu spôsobu výroby tzv. Pidgeon procesom.

Na projekte, ktorý bol financovaný americkým ministerstvom energetiky (US Dept. of Energy) prostredníctvom ARPA-E (Advance Research Project Agency - Energy) spolupracovali nasledujúce inštitúcie: Valparaiso University, Valparaiso, Indiana; Purdue University, West Lafayette, Indiana; Navigant, Chicago, Ústav anorganickej chémie SAV a Diver Solar Albuquerque, Nové Mexiko. Projekt v súčasnosti konvertoval do tzv. up-scale testu (1000 A, 1000 hodín), ktorý financuje US DOE a realizuje sa v Materials and Electrochemical Corporation, Tuscon, Arizona.



Obr: Schéma procesu: elektrochemická reakcia výroby Mg za použitia solárneho tepelného inputu. Tepelný input je maximálny pri minimálnom napätí. Na pravej strane závislosť prúdu od napätia. Elektrolyt: $(MgF_2 - CaF_2)_{EUT} - MgO(sat)$, katóda: Mo, anóda: grafit. Napätie je definované ako rozdiel medzi aktuálnym napätím a vertikálou ktorá reprezentuje termodynamický vylučovací potenciál 1.38 V.

LEONARD, N. – KORENKO, Michal – LARSON, C. – BLOOD, K. – VENSTROM, Luke J. – NUDEHI, S. – DUNCAN, S. – DIVER, R. – ŠIMKO, František – PRIŠČÁK, Jozef – SCHOER, J. – KISSINGER, P.T. – PALUMBO, R. The thermal electrolytic production of Mg from MgO: A discussion of the electrochemical reaction kinetics and requisite mass transport processes. In Chemical Engineering Science, 2016, vol. 148, p. 155-169. (2.750 – IF2015). Typ: ADCA

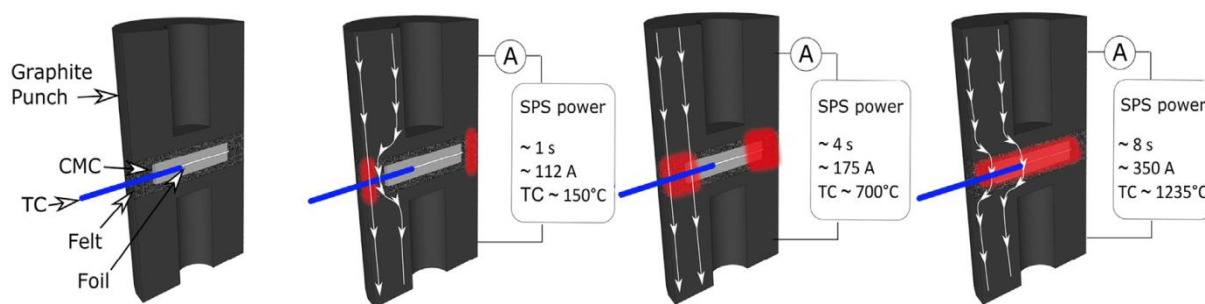
KORENKO, Michal – LARSON, C. – BLOOD, K. – PALUMBO, R. – NUDEHI, S. – DIVER, R. – BLOOD, D. – ŠIMKO, František – VENSTROM, Luke J. Technical and economic evaluation of a solar thermal MgO electrolysis process for magnesium production. In Energy, 2017, vol. 135, p. 182-194. (4.520 – IF2016). ISSN 0360-5442. Typ: ADCA

Ultrarýchle spájanie povlakovaných (CVD-SiC) vláknitých keramických kompozitov Cf/SiC s medzivrstvou Ti

Peter Tatarko, Pavol Šajgalík

Tento výskum po prvýkrát popisuje vývoj novej technológie spájania, tzv. “Flash joining”, pri ktorej je elektrický prúd počas procesu spekania priamo vedený cez spájané materiály. Najlepšia pevnosť v šmyku, ktorá sa rovnala pevnosti základného materiálu, bola dosiahnutá pri spájaní vzoriek počas 8 sekúnd s odpovedajúcou maximálnou teplotou 1237°C. Veľmi vysoká rýchlosť ohrevu (9 600°C/min) a veľmi krátky čas procesu (~ 8 s) potlačil difúzne procesy medzi základnými materiálmi a medzivrstvou. Výsledkom bol nový mechanizmus spájania, ktorý pozostával z tvorby spoja na kovovej báze (Ti), pričom absencia akejkoľvek detekovateľnej reakčnej fázy výrazne znížila dobu potrebnú pre difúzne spájanie v tuhej fáze. V porovnaní so štandardnými procesmi spájania (s typickou dobou ~ 1 hod a teplotou ~ 1700°C) táto novovyvinutá

metóda „flash joining“ predstavuje výrazné skrátenie celého procesu spájania (~ 8 s) a zníženie teploty spájania ($\sim 1250^{\circ}\text{C}$).



Obr. Schématické zobrazenie novovyvinutej metodiky spájania, tzv. „flash joining“

TATARKO, Peter - GRASSO, Salvatore - SAUNDERS, Theo G. - FERRARIS, Monica - REECE, Michael J. **Flash joining of CVD-SiC coated Cf/SiC composites with a Ti interlayer**. In Journal of the European Ceramic Society, 2017, vol. 37, no. 13, p. 3841-3848. (3.411 - IF2016). ISSN 0955-2219

Práca vznikla v rámci riešenia medzinárodného **EU projektu** v programe **FP7 2007-2013** pod názvom „**ADMACOM**“ – Advanced manufacturing routes for metal/composite components for aerospace, č. 609188. Niektoré experimenty a s tým spojené aktivity boli taktiež financované národným projektom „**Extremecer**“ pod číslom **APVV-15-0469**.

2.4. Publikačná činnosť (zoznam je uvedený v prílohe C)

Tabuľka 2e Štatistika vybraných kategórií publikácií

PUBLIKAČNÁ A EDIČNÁ ČINNOSŤ	Počet v r. 2017/ doplňky z r. 2016
1. Vedecké monografie a monografické štúdie vydané v domácich vydavateľstvách (AAB, ABB)	0 / 0
2. Vedecké monografie a monografické štúdie vydané v zahraničných vydavateľstvách (AAA, ABA)	1 / 0
3. Odborné monografie, vysokoškolské učebnice a učebné texty vydané v domácich vydavateľstvách (BAB, ACB, CAB)	0 / 0
4. Odborné monografie a vysokoškolské učebnice a učebné texty vydané v zahraničných vydavateľstvách (BAA, ACA, CAA)	0 / 0
5. Kapitoly vo vedeckých monografiách vydaných v domácich vydavateľstvách (ABD)	0 / 0
6. Kapitoly vo vedeckých monografiách vydaných v zahraničných vydavateľstvách (ABC)	5 / 0
7. Kapitoly v odborných monografiách, vysokoškolských učebniciach a učebných textoch vydaných v domácich vydavateľstvách (BBB, ACD)	0 / 0
8. Kapitoly v odborných monografiách, vysokoškolských učebniciach a učebných textoch vydaných v zahraničných vydavateľstvách (BBA, ACC)	0 / 0
9. Vedecké práce registrované v Current Contents Connect (ADCA, ADCB, ADDA, ADDB)	48 / 1
10. Vedecké práce registrované vo Web of Science Core Collection alebo Scopus (ADMA, ADMB, ADNA, ADN B)	3 / 0
11. Vedecké práce v ostatných domácich časopisoch (ADFA, ADFB)	1 / 0
12. Vedecké práce v ostatných zahraničných časopisoch (ADEA, ADEB)	0 / 0
13. Vedecké práce v domácich recenzovaných zborníkoch (AEDA)	2 / 0
14. Vedecké práce v zahraničných recenzovaných zborníkoch (AECA)	0 / 0
15. Publikované príspevky na domácich vedeckých konferenciách (AFB, AFD)	8 / 0
16. Publikované príspevky na zahraničných vedeckých konferenciách (AFA, AFC)	5 / 0
17. Vydané periodiká evidované v CCC, WoS Core Collection, SCOPUS	0
18. Ostatné vydané periodiká	0
19. Zostavovateľské práce knižného charakteru (FAI)	1 / 0
20. Preklady vedeckých a odborných textov (EAJ)	0 / 0
21. Heslá v odborných terminologických slovníkoch a encyklopédiách (BDA, BDB)	0 / 1
22. Recenzie v časopisoch a zborníkoch (EDI)	0 / 0

Evidujú len tie práce zamestnancov a doktorandov, v ktorých je uvedená afiliácia k organizácii

Tabuľka 2f Štatistika vedeckých prác podľa kvartilu vedeckého časopisu

Kvartil vedeckého časopisu	Q1	Q2	Q3	Q4	Spolu
Podľa IF z r. 2016 (zdroj JCR) <i>Počet článkov / doplnky 2015</i>	30 / 0	11 / 1	5 / 0	4 / 0	50 / 1
Podľa SJR z r. 2016 (zdroj Scimago) <i>Počet článkov / doplnky 2015</i>	36 / 1	8 / 0	6 / 0	1 / 0	51 / 1

Tabuľka 2g Ohlasy

OHLASY	Počet v r. 2016/ doplnky z r. 2015
Citácie vo WOS (1.1, 2.1)	1366 / 5
Citácie v SCOPUS (1.2, 2.2)	18 / 98
Citácie v iných citačných indexoch a databázach (9, 10, 3.2, 4.2)	0 / 0
Citácie v publikáciách neregistrovaných v citačných indexoch (3, 4, 3.1, 4.1)	1 / 0
Recenzie na práce autorov z organizácie (5, 6, 7, 8)	0 / 0

2.5. Aktívna účasť na vedeckých podujatiach

Tabuľka 2h Vedecké podujatia

Prednášky a vývesky na medzinárodných vedeckých podujatiach	59
Prednášky a vývesky na domácich vedeckých podujatiach	20

2.6. Vyžiadané prednášky

2.6.1. Vyžiadané prednášky na medzinárodných vedeckých podujatiach

- 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, Turecko, 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, Rakúsko, 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, Nemecko, 4. 9. 2017
- Z. LENČEŠ, I. IBRAHIM, P. ŠAJGALÍK, E. BENCO**. Experimental and theoretical approach to lanthanide-doped LaSi3N5 phosphors. 41st International Conference and Exposition on Advanced Ceramics and Composites (ICACC 2017), January 22 - 27, 2017, Hilton Daytona Beach Resort and Ocean Center, Daytona Beach, Florida, USA.
- O. MALKIN**, How to analyze the hyperfine deformation density? Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Rakúsko, 7.3-9.3.2017
- 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, Japonsko, 8-9.12.207
- V. MALKIN**, Visualization of EPR hyperfine coupling pathways. Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Rakúsko, 7.3-9.3.2017
- 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,

Japonsko, 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)

E. SCHOLTZOVA, Problematic Parts of IR Spectrum and Stability of Organoclays - DFT Study. AnalytiX-2017, Fukuoka, Japonsko, 23.3.2017

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

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), May 21 - 26, 2017, Waikoloa, Hawaii, USA.

P. ŠAJGALÍK, **M. HNATKO**, **Z. LENČEŠ**, **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), May 21 - 26, 2017, Waikoloa, Hawaii, USA.

P. ŠAJGALÍK, **M. HNATKO**, **Z. LENČEŠ**, **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), January 22 - 27, 2017, Hilton Daytona Beach Resort and Ocean Center, Daytona Beach, Florida, USA.

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), January 22 - 27, 2017, Hilton Daytona Beach Resort and Ocean Center, Daytona Beach, Florida, USA.

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), July 26-28, 2017, University of Trento, Italy.

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

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

P. ŠAJGALÍK, **Z. LENČEŠ**, 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), August 27 - 31, 2017, Hokkaido University, Sapporo, Japan, pp. 129.

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

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

2.6.2. Vyžiadané prednášky na domácich vedeckých podujatiach

P. BOHÁČ, Vplyv teploty na absorpčné spektrá hybridných systémov vrstevnatých silikátov s organickými farbivami. Workshop Aplikácie v UV-Vis-NIR spektrofotometrii. Bratislava, 26. 9. 2017

P. BOHÁČ, Vplyv teploty na fotofyzikálne vlastnosti látok. Možnosti využitia UV-VIS-NIR spektroskopie. Seminár HERMES, Košice, 3.10.2017, Bratislava 5.10.2017

J. BUJDÁK, Využitie metachromatizmu farbív pre detekciu a charakterizáciu ílových minerálov. 4. seminár Slovenskej ílovej spoločnosti, Stará Lesná, 19. 6. 2017

J. BUJDÁK, Využitie metachromatizmu farbív pre detekciu a charakterizáciu koloidných častíc vrstevnatých silikátov. Workshop Aplikácie v UV-Vis-NIR spektrofotometrii. Bratislava, 26. 9. 2017

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

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

2.6.3. Vyžiadané prednášky na významných vedeckých inštitúciách

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

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

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

T. BUČKO, Enthalpy, entropy, and confinement: a DFT modelling beyond static approach, seminár, IFP Energies nouvelles (IFPEN) Lyon, Francúzsko, 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 ReSpec program, Helmholtz-Zentrum Dresden-Rossendorf: Chemistry of the f-elements, Drážďany, Nemecko, 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, Berlín, Nemecko, 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, Peking, Čína, 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, Šanghaj, Čína, 23.05.2017
- Northeastern University, Shenyang, Čína, 25.05.2017

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

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

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

Ak boli príspevky publikované, sú súčasťou prílohy C, kategória (AFC, AFD, AFE, AFF, AFG, AFH)

2.7. Patentová a licenčná činnosť na Slovensku a v zahraničí v roku 2017**2.7.1. Vynálezy, na ktoré bol udelený patent****2.7.2. Prihlásené vynálezy****2.7.3. Predané licencie****2.7.4. Realizované patenty**

Finančný prínos pre organizáciu SAV v roku 2017 a súčet za predošlé roky sa neuádzajú, ak je zverejnenie v rozpore so zmluvou súvisiacou s realizáciou patentu.

2.8. Účasť expertov na hodnotení národných projektov (APVV, VEGA a iných)

Tabuľka 2i Experti hodnotiaci národné projekty

Meno pracovníka	Typ programu/projektu/výzvy	Počet hodnotených projektov
Galusek Dušan	APVV SK-FR 2017	1
	APVV VV2016	1
	VEGA 201	1
Hnatko Miroslav	APVV VV	1
	VEGA	2
Jankovič Ľuboš	APVV SK-FR 2017	1
	APVV VV	1
	SK-AT-2017-0017	1
	SK-CN-2017-0024	1
Lencéš Zoltán	VEGA	5
Sedláček Jaroslav	VEGA	2
Tatarko Peter	VEGA	1

2.9. Účasť na spracovaní hesiel do encyklopédie Beliana

Počet autorov hesiel: 0

2.10. Recenzovanie publikácií a príspevkov vo vedeckých časopisoch

Tabuľka 2j Počet recenzovaných monografií, článkov, zborníkov

Meno pracovníka	Knížné monografie		Príspevky v časopisoch			Zborníky	
	Domáce	Zahra-ničné	WoS, SCOPUS	Iné databázy	Ostatné	Domáce	Zahra-ničné
Boča Miroslav	0	0	3	0	0	0	0
Bujdák Juraj	0	0	12	0	0	0	0
Galusek Dušan	0	0	2	0	0	0	0
Hnatko Miroslav	0	0	1	0	0	1	0
Kubíková Blanka	0	0	3	0	0	0	0
Lencéš Zoltán	0	0	4	0	0	0	0
Madejová Jana	0	0	2	0	0	0	0

Malkin Oľga	0	0	3	0	0	0	0
Malkin Vladimír	0	0	1	0	0	0	0
Pálková Helena	0	0	1	0	0	0	0
Pavlík Viliam	0	0	1	0	0	0	0
Scholtzová Eva	0	0	2	0	0	0	0
Spolu	0	0	35	0	0	1	0

2.11. Iné informácie k vedeckej činnosti.

Počet časopiseckých impaktovaných publikácií registrovaných v databáze WOS a SCOPUS v roku 2017 dosiahol číslo 53. V závislosti na metodike, na ktorú kategóriu vzťahnúť prepočítaný podiel publikácie, je možné uvažovať o kategóriách: vedeckí pracovníci, ostatní vedeckí pracovníci s VŠ vzdelaním, ostatní pracovníci zapojení do riešenia projektov a doktorandi. Vzhľadom na to, že nie je k dispozícii jednoznačné usmernenie, budeme vychádzať z usmernenia poslednej akreditácie, kedy sa počet publikačných výstupov vzťahoval na počet zamestnancov s univerzitným titulom zapojených do výskumných projektov 44,3, vrátane šiestich doktorandov, ktorí k 31.12. vystupovali v riešiteľských kolektívoch 50,3. Potom na jedného pracovníka pripadá 1,2 publikácie, vrátane doktorandov - 1,1 publikácie.

Takýto stav považujeme za neuspokojivý a cieľom ostáva dosiahnuť dve publikácie na vedeckého pracovníka ročne, ktorý zodpovedá štandardu vyspelých vedeckých pracovísk s podobným zameraním. Priemerný impakt faktor časopisov, v ktorých boli práce uverejnené, bol 2,83, pokiaľ vlani to bolo 2,71 (treba mať na pamäti, že údaje sú so záverečných správ, v ktorých sa nachádzajú aj doplnky publikácií za predchádzajúci rok, ako aj chýbajúce publikácie za rok 2017, ktorým ešte neboli priradené kompletne bibliografické údaje). Citovanosť (vo všetkých dostupných databázach WOS – 1356, SCOPUS – 116) na vedeckého pracovníka (39,1) je 37,6 citácií, čo predstavuje len veľmi mierny nárast v porovnaní s rokom 2016. Pracovníci ústavu predniesli 22 pozvaných prednášok na významných svetových konferenciách.

3. Doktorandské štúdium, iná pedagogická činnosť a budovanie ľudských zdrojov pre vedu a techniku

3.1. Údaje o doktorandskom štúdiu

Tabuľka 3a Počet doktorandov v roku 2017

Forma	Počet k 31.12.2017						Počet ukončených doktorantúr v r. 2017					
	Doktorandi						Ukončenie z dôvodov					
	celkový počet		z toho novoprijatí		po skúške		ukončenie úspešnou obhajobou		predčasné ukončenie		neúspešné ukončenie	
	M	Ž	M	Ž	M	Ž	M	Ž	M	Ž	M	Ž
Denná zo zdrojov SAV	5	1	2	1	2	0	1	0	0	1	0	0
Denná z iných zdrojov	0	0	0	0	0	0	0	0	0	0	0	0
Externá	0	0	0	0	0	0	1	0	0	1	0	0
Spolu	5	1	2	1	2	0	2	0	0	2	0	0
Súhrn	6		3		2		2		2		0	

Uvádzajte len doktorandov organizácie ako externej vzdelávacej inštitúcie

3.2. Zmena formy doktorandského štúdia

Tabuľka 3b Počty preradení z dennej formy na externú a z externej na dennú

Pôvodná forma	Denná z prostriedkov SAV	Denná z prostriedkov SAV	Denná z iných zdrojov	Denná z iných zdrojov	Externá	Externá
Nová forma	Denná z iných zdrojov	Externá	Denná z prostriedkov SAV	Externá	Denná z prostriedkov SAV	Denná z iných zdrojov
Počet	0	0	0	0	0	0

3.3. Zoznam doktorandov, ktorí ukončili doktorandské štúdium úspešnou obhajobou

Tabuľka 3c Menný zoznam ukončených doktorandov v roku 2017 úspešnou obhajobou

Meno doktoranda	Forma DŠ	Mesiac, rok nástupu na DŠ	Mesiac, rok obhajoby	Číslo a názov študijného odboru	Meno a organizácia školiteľa	Fakulta udeľujúca vedeckú hodnosť
Mgr. Lukáš Petra	interné štúdium hrazené z prostriedkov	9 / 2013	8 / 2017	4.1.15 anorganická chémia	RNDr. Peter Komadel DrSc., Ústav anorganickej chémie SAV	Prírodovedecká fakulta UK

Ing. Michal Šimurda	kov SAV externé štúdium	9 / 2012	8 / 2017	5.2.19 anorganická technológia a materiály	doc. Ing. Miroslav Boča DrSc., Ústav anorganickej chémie SAV	Fakulta chemickej a potravinárskej technológie STU
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Zoznam interných a externých doktorandov je uvedený v prílohe A.

3. 4. Medzinárodné doktorandské štúdium

Tabuľka 3d Počet študentov v medzinárodných programoch doktorandského štúdia

Cotutelle	Co-direction	Iné	Zahraniční doktorandi
0	0	0	1

3.5. Zoznam akreditovaných študijných odborov s uvedením VŠ

Tabuľka 3e Zoznam akreditovaných študijných odborov s uvedením univerzity/vysokej školy a fakulty, kde sa doktorandský študijný program uskutočňuje

Názov študijného odboru (ŠO)	Číslo ŠO	Doktorandské štúdium uskutočňované na (univerzita/vysoká škola a fakulta)
chemická fyzika	4.1.11	Prírodovedecká fakulta UK
anorganická chémia	4.1.15	Prírodovedecká fakulta UK
anorganická technológia a materiály	5.2.19	Fakulta chemickej a potravinárskej technológie STU
anorganická technológia a materiály	5.2.19	Slovenská technická univerzita v Bratislave

Tabuľka 3f Účasť na pedagogickom procese

Menný prehľad pracovníkov, ktorí boli menovaní do spoločných odborových komisií pre doktorandské štúdium	Menný prehľad pracovníkov, ktorí pôsobili ako členovia vedeckých rád univerzít, správnych rád univerzít a fakúlt	Menný prehľad pracovníkov, ktorí získali vyššiu vedeckú, pedagogickú hodnotu alebo vyšší kvalifikačný stupeň
doc. Ing. Miroslav Boča, DrSc. (anorganická chémia)	doc. Ing. Miroslav Boča, DrSc. (Trenčianska univerzita Alexandra Dubčeka v Trenčíne)	Mgr. Stanislav Komorovský, PhD. (IIa)
doc. Ing. Miroslav Boča, DrSc. (anorganická technológia a materiály)	prof. Ing. Dušan Galusek, DrSc. (Fakulta špeciálnej techniky TnUAD)	Ing. Anna Prnová, PhD. (IIa)
doc. RNDr. Juraj Bujdák, DrSc. (anorganická chémia)	prof. Ing. Dušan Galusek, DrSc. (Fakulta zdravotníctva TnUAD)	Mgr. Silvia Belušáková, PhD. (PhD., Prírodovedecká fakulta UK)
doc. RNDr. Juraj Bujdák, DrSc. (fyzikálna chémia)	prof. Ing. Dušan Galusek, DrSc. (Trenčianska univerzita Alexandra Dubčeka v Trenčíne)	
prof. Ing. Dušan Galusek, DrSc. (anorganická technológia a materiály)	prof. Ing. Marek Liška, DrSc. (Fakulta chemické technologie VŠCHT, Praha, ČR)	
doc. Ing. Miroslav Hnatko, PhD.	prof. Ing. Marek Liška, DrSc.	

(anorganická technológia a materiály)	(Trenčianska univerzita Alexandra Dubčeka v Trenčíne)
RNDr. Peter Komadel, DrSc. (anorganická chémia)	prof. RNDr. Jozef Noga, DrSc. (Fakulta prírodných vied UMB)
doc. Ing. Zoltán Lenčoš, PhD. (anorganická technológia a materiály)	prof. RNDr. Jozef Noga, DrSc. (Prírodovedecká fakulta UK)
doc. Ing. Zoltán Lenčoš, PhD. (anorganická chémia)	prof. RNDr. Pavol Šajgalík, DrSc. (Fakulta metalurgie a materiálového inžinierstva, Vysoká škola báňská TU)
doc. Ing. Zoltán Lenčoš, PhD. (odbor v zahraničí)	prof. RNDr. Pavol Šajgalík, DrSc. (Hutnícka fakulta TUKE)
prof. Ing. Marek Liška, DrSc. (anorganická technológia a materiály)	prof. RNDr. Pavol Šajgalík, DrSc. (Slovenská technická univerzita v Bratislave)
prof. Ing. Marek Liška, DrSc. (fyzika kondenzovaných látok a akustika)	prof. RNDr. Pavol Šajgalík, DrSc. (Trenčianska univerzita Alexandra Dubčeka v Trenčíne)
RNDr. Jana Madejová, DrSc. (anorganická technológia a materiály)	prof. RNDr. Pavol Šajgalík, DrSc. (Univerzita Komenského v Bratislave)
Dr. Oľga Malkin, DrSc. (teoretická a počítačová chémia)	prof. RNDr. Pavol Šajgalík, DrSc. (Univerzita Pavla Jozefa Šafárika v Košiciach)
Dr. Vladimír Malkin, DrSc. (chemická fyzika)	prof. RNDr. Pavol Šajgalík, DrSc. (Univerzita sv. Cyrila a Metoda v Trnave)
Dr. Vladimír Malkin, DrSc. (teoretická a počítačová chémia)	prof. RNDr. Pavol Šajgalík, DrSc. (Vysoké učení technické, Brno)
prof. RNDr. Jozef Noga, DrSc. (chemická fyzika)	
prof. RNDr. Jozef Noga, DrSc. (anorganická chémia)	
prof. RNDr. Jozef Noga, DrSc. (fyzika plazmy)	

3.6. Údaje o pedagogickej činnosti

Tabuľka 3g Prednášky a cvičenia vedené v roku 2017

PEDAGOGICKÁ ČINNOSŤ	Prednášky		Cvičenia a semináre	
	doma	v zahraničí	doma	v zahraničí
Počet prednášateľov alebo vedúcich cvičení	4	1	4	0
Celkový počet hodín v r. 2017	12	60	237	0

Prehľad prednášateľov predmetov a vedúcich cvičení, s uvedením názvu predmetu, úväzku, katedry, fakulty, univerzity/vysokej školy je uvedený v prílohe D.

Tabuľka 3h Aktivity pracovníkov na VŠ

1. Počet pracovníkov, ktorí pôsobili ako vedúci alebo konzultanti diplomových a bakalárskych prác	2
2. Počet vedených alebo konzultovaných diplomových a bakalárskych prác	2

3. Počet pracovníkov, ktorí pôsobili ako školitelia doktorandov (PhD.)	14
4. Počet školených doktorandov (aj pre iné inštitúcie)	25
5. Počet oponovaných dizertačných a habilitačných prác	9
6. Počet pracovníkov, ktorí oponovali dizertačné a habilitačné práce	7
7. Počet pracovníkov, ktorí pôsobili ako členovia komisií pre obhajoby DrSc. prác	1
8. Počet pracovníkov, ktorí pôsobili ako členovia komisií pre obhajoby PhD. prác	10
9. Počet pracovníkov, ktorí pôsobili ako členovia komisií, resp. oponenti v inauguračnom alebo habilitačnom konaní na vysokých školách	1

3.7. Iné dôležité informácie k pedagogickej činnosti

ÚACH SAV vypísal pre akademický rok 2017/2018 celkovo 15 tém pre doktorandské štúdium vo všetkých akreditovaných odboroch: 4.1.15 Anorganická chémia, 5.2.19 Anorganické technológie a materiály a 4.1.11 Chemická fyzika. Po úspešnom prijímacom konaní nastúpili traja noví študenti na internú formu doktorandského štúdia v študijnom odbore 5.2.19 Anorganické technológie a materiály na FCHPT STU.

V akademickom roku 2016/2017 obhájili dizertačné práce dvaja študenti: Mgr. Lukáš Petra v študijnom odbore 4.1.15 Anorganická chémia (denná forma) a Ing. Michal Šimurda v študijnom odbore 5.2.19 Anorganické technológie a materiály (externá forma).

PhD študenti na ÚACH SAV sa pravidelne zúčastňujú na študentských vedeckých podujatiach a konferenciách, akými sú napr. ŠVK FCHPT STU 2017.

Dňa 06.10.2017 sa na ÚACH SAV konala Súťaž mladých vedeckých pracovníkov do 35 rokov za účasti 11 mladých vedeckých pracovníkov z ÚACH SAV Bratislava a z Tn AD Trenčín. Na prvých troch miestach sa umiestnili:

1.miesto: Ing. Silvia Belušáková, PhD. a Ing. Ondrej Hanzel, PhD.,

2.miesto: Ing. Martin Barlog,

3.miesto: Ing. Alexandra Nowicka.

Dvaja najúspešnejší účastníci (Ing. Silvia Belušáková, PhD. a Ing. Ondrej Hanzel, PhD.) sa dňa 25.10.2017 zúčastnili podobnej súťaže na Ústave anorganickej chémie ČAV v Řeži, na ktorej Ing. Silvia Belušáková, PhD. obsadila delené prvé miesto.

Doc. Ing. Zoltán Lenčoš, PhD. a doc. Ing. Miroslav Hnatko, PhD. pôsobili roku 2017 ako školitelia-spezialisti troch zahraničných študentiek (Christina Atzenhofer, Anastasia Kucheryavaya a Taťána Fenclová), ktoré si v rámci vzájomnej spolupráce s Montanuniversität Leoben, Austria, resp. VŠB-Technická univerzita Ostrava, realizovali časť svojich PhD. prác na ÚACH SAV. V rámci programu Erasmus, doktorandka Lenka Bláhová z Prírodovedeckej fakulty Ostravskej univerzity absolvovala na ústave trojmesačnú stáž zameranú na analýzu rôzne modifikovaných vysokopecných trosiek.

4. Medzinárodná vedecká spolupráca

4.1. Medzinárodné vedecké podujatia

4.1.1. Medzinárodné vedecké podujatia, ktoré organizácia SAV organizovala v roku 2017 alebo sa na ich organizácii podieľala, s vyhodnotením vedeckého a spoločenského prínosu podujatia

10th Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Rakúsko, 56 účastníkov, 05.03.-10.03.2017

Počas podujatia odznelo 28 prednášok. Konferencie sa zúčastnili vedeckí pracovníci z Nemecka, Francúzska, Českej republiky, Dánska, Fínska, Japonska a Slovenska.

4.1.2. Medzinárodné vedecké podujatia, ktoré usporiada organizácia SAV v roku 2018 (anglický a slovenský názov podujatia, miesto a termín konania, meno, telefónne číslo a e-mail zodpovedného pracovníka)

11th Workshop on Modern Methods in Quantum Chemistry/11th Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Rakúsko, 25.02.-02.03.2018, (Vladimír Malkin, 02/59410469, uachmalk@savba.sk)

4.1.3. Počet pracovníkov v programových a organizačných výboroch medzinárodných konferencií

Tabuľka 4a Programové a organizačné výbory medzinárodných konferencií

Meno pracovníka	Programový	Organizačný	Programový i organizačný
Boča Miroslav	1	0	0
Galusek Dušan	0	0	1
Lenčేశ Zoltán	0	0	1
Malkin Vladimír	0	0	1
Šajgalík Pavol	5	0	0
Spolu	6	0	3

4.2. Členstvo a funkcie v medzinárodných orgánoch

4.2.1. Členstvo a funkcie v medzinárodných vedeckých spoločnostiach, úniách a národných komitétach SR

Mgr. Silvia Belušáková, PhD.

AIPEA - International Association for the study of Clays (funkcia: člen)

Mgr. Valéria Bizovská, PhD.

AIPEA - International Association for the study of Clays (funkcia: člen)

doc. Ing. Miroslav Boča, DrSc.

European Technology Platform for Advanced Engineering Materials and Technologies (funkcia: člen správnej rady EuMat)

Mgr. Peter Boháč, PhD.

AIPEA - International Association for the study of Clays (funkcia: člen)

doc. RNDr. Juraj Bujdák, DrSc.

AIPEA - International Association for the study of Clays (funkcia: člen)

Mgr. Adriana Czímerová, PhD.

AIPEA - International Association for the study of Clays (funkcia: člen)

prof. Ing. Dušan Galusek, DrSc.

American Ceramic Society (funkcia: člen)

European Society on Glass Science and Technology (funkcia: člen)

Mgr. Ľuboš Jankovič, PhD.

AIPEA - International Association for the study of Clays (funkcia: člen)

RNDr. Peter Komadel, DrSc.

AIPEA - International Association for the study of Clays (funkcia: člen)

The Clay Minerals Society (funkcia: člen)

Ing. Michal Korenko, PhD.

International Union of Pure and Applied Chemistry (IUPAC) (funkcia: National Representative (NR) of Division I)

doc. Ing. Zoltán Lenčéš, PhD.

American Ceramic Society (funkcia: člen)

Ceramic Society of Japan (funkcia: člen)

Council of the European Ceramic Society (funkcia: člen)

European Ceramic Society (funkcia: člen)

International Ceramic Federation (funkcia: člen)

Materials Research Society (funkcia: člen)

RNDr. Jana Madejová, DrSc.

AIPEA - International Association for the study of Clays (funkcia: člen výboru)

The Clay Minerals Society (funkcia: člen)

Dr. Vladimír Malkin, DrSc.

WATOC - World Association of Theoretical and Computational Chemists (funkcia: člen)

Mgr. Marián Matejdes, PhD.

AIPEA - International Association for the study of Clays (funkcia: člen)

prof. RNDr. Jozef Noga, DrSc.

International Academy of Quantum Molecular Sciences (funkcia: volený člen)

World Association of Theoretical and Computational Chemists (funkcia: člen)

Ing. Helena Pálková, PhD.

AIPEA - International Association for the study of Clays (funkcia: člen)

Ing. Eva Scholtzová, CSc.

AIPEA - International Association for the study of Clays (funkcia: člen)

Ing. Michal Slaný

AIPEA - International Association for the study of Clays (funkcia: člen)

prof. RNDr. Pavol Šajgalík, DrSc.

American Ceramic Society (funkcia: člen)

Ceramic Society of Japan (funkcia: člen)

Council of the European Ceramic Society (funkcia: člen)

ECerS (funkcia: prezident)

International Ceramic Federation (funkcia: člen predstavenstva)

Materials Research Society (funkcia: člen)

Permanent Executive Committee ECerS (funkcia: volený člen)

World Academy of Ceramics (funkcia: volený člen)

World Academy of Ceramics - Člen výkonného výbor (funkcia: volený člen)

doc. Ing. Peter Šimurka, PhD.

European Society on Glass Science and Technology (funkcia: člen)

International Commission on Glass (funkcia: výkonný tajomník)

4.3. Účasť expertov na hodnotení medzinárodných projektov (EÚ RP, ESF a iných)

Tabuľka 4b Experti hodnotiaci medzinárodné projekty

Meno pracovníka	Typ programu/projektu/výzvy	Počet hodnotených projektov
Lenčes Zoltán	MAD, Bilaterálne mobilitné projekty ČR-SK	1
Sedláček Jaroslav	COST	1

4.4. Najvýznamnejšie prínosy MVTS ústavu vyplývajúce z mobility a riešenia medzinárodných projektov a iné informácie k medzinárodnej vedeckej spolupráci

Valéria Bizovská

- Jerzy Haber Institute of Catalysis and Surface Chemistry PAS, Krakow, Poľsko (15. – 25. 10. 2017). Experimentálne práce v rámci spoločného projektu „Immobilization of metal nanoparticles on organo-modified layered silicates”. Medziakademická spolupráca (MAD) medzi Ústavom anorganickej chémie SAV a ústavom PAV.

Miroslav Boča

- Shanghai Institute of Applied Physics, Chinese Academy of Science, Šanghaj, Čína (21.-24.05. 2017). Medziakademická spolupráca (MAD) medzi Ústavom anorganickej chémie SAV a ústavom čínskej AV. Dňa 23.05.2017 prednášky s názvom Molten salts: from fundamental research to hydrogen economy a XPS and NMR spectroscopy of ternary fluorides.
- Northeastern University, Shenyang, Čína (24.-26.05. 2017). Spoločný projekt “Nové technológie pri výrobe hliníka - Fyzikálno-chemické a elektrochemické skúmanie sľubných draselných kryolitových sústav”. Bilaterálny projekt SK-CN-2015-0014 medzi Ústavom anorganickej chémie SAV a Northeastern University. Dňa 25.05.2017 prednášky s názvom Molten salts: from fundamental research to hydrogen economy a XPS and NMR spectroscopy of ternary fluorides.
- Northeastern University, Shenyang, Čína (26.11.-6.12.2017). Pobyt sa uskutočnil na základe pozvania z čínskej strany a jeho účelom bola výučba Teórie chemickej väzby pre vybranú skupinu študentov z Northeastern University v Shenyangu.

Stanislav Komorovský

- CTCC, Department of Chemistry, University of Tromsø, Tromsø, Nórsko (27.01 - 06.02.2017), v rámci projektu SASPRO 1563/03/02. V skupine Kennetha Ruuda sme pracovali na príprave zverejnenia ReSpect kódu. Konkrétne sme implementovali novú schému na kompiláciu (autocmake) a pripravili sme novú schému na čítanie vstupov a prenosu dát pre jednotlivé výpočtové moduly.
- Institut für Chemie, Technische Universität Berlin, Nemecko (22.06-29.06.2017), v rámci projektu VEGA 2/0116/17. V rámci cesty som prezentoval najnovší vývoj relativistických metód v programe ReSpect, za cieľom rozšírenia spolupráce so skupinou profesora Martina Kauppa. Takisto som vyriešil problém s inštaláciou ReSpect programu na výpočtovom klastry v Berlíne.
- Helmholtz-Zentrum Dresden-Rossendorf: Chemistry of the f-elements, Drážďany, Nemecko (05.06-10.06.2017), v rámci projektu SASPRO 1563/03/02. V rámci cesty som prezentoval vývoj TDDFT metódy v programe ReSpect na seminári s názvom “Development of open-shell TDDFT method within four-component domain in ReSpect program”.
- Institut für Chemie, Technische Universität Berlin, Berlín, Nemecko (06.09-12.09.2017), v rámci projektov APVV-15-0726 a SASPRO 1563/03/02. V skupine Martina Kauppa som odprednášal seminár “Recent advances in the calculation of excitation energies in the framework of fully relativistic TDDFT theory”.
- Department of Materials Research and Physics; Chemistry of Materials, University of Salzburg,

Salzburg, Rakúsko (01.10-05.10.2017), v rámci projektu DS-2016-0009 (GOLDCAT). V rámci cesty sme diskutovali s Raphaelom Bergerom na možnostiach spolupráce v oblasti analýzy Spin-Orbitálnej interakcie k NMR chemickému posunu.

Michal Korenko

- Massachusetts Institute of Technology, Cambridge, USA (7.-10.3. 2017). Diskusia o možnej spolupráci medzi OTS ÚACH SAV a skupinou Prof. Ch. Forsberga v oblasti taveninových jadrových reaktorov. Predstavenie nášho ústavu s dôrazom na vysokoteplotnú a taveninovú chémiu.
- Wisconsin University Madison, Madison, USA (22.-24. 3. 2017) Návšteva v rámci zahraničnej služobnej cesty. Prednáška s názvom Molten Fluoride Science in Slovakia. Diskusia o spolupráci medzi OTS ÚACH SAV a skupinou Dr. R. Scarlat a skupinou Dr. K. Sridharan v oblasti taveninových jadrových reaktorov s dôrazom na koróziu konštrukčných materiálov v taveninách a s tým súvisiacej kontroly redox potenciálu.
- Venture Café Foundation Boston, USA (3.-16.7.2017). Séria prednášok úspešných start-upov a projektov financovaných US Dept. of Energy.
- Institute of High Energy Physics, Čínska Akadémia Vied, Peking, Čína (14.-28.8. 2017) Medziakademická spolupráca (MAD) medzi Ústavom anorganickej chémie SAV a ústavom čínskej AV. Dňa 24.08.2017 prednášky s názvom Solar Thermal Electrolysis of Mg from molten Fluorides.

Blanka Kubíková

- Shanghai Institute of Applied Physics, Chinese Academy of Science, Šanghaj, Čína (21.-24.05. 2017). Medziakademická spolupráca (MAD) medzi Ústavom anorganickej chémie SAV a ústavom čínskej AV. Prednáška: Physico-chemical properties of molten systems based on lanthanum fluoride (23.5.2017).
- Northeastern University, Shenyang, Čína (24.-26.05. 2017). Spoločný projekt "Nové technológie pri výrobe hliníka - Fyzikálno-chemické a elektrochemické skúmanie sľubných draselných kryolitových sústav". Bilaterálny projekt SK-CN-2015-0014 medzi Ústavom anorganickej chémie SAV a Northeastern University. Prednášky: Physico-chemical properties of molten systems based on lanthanum fluoride a Physico-chemical investigation of potassium cryolite molten systems (25.5.2017).

Oľga Malkin

- Paris-Lodron Universität Salzburg (7. – 11.9. 2017) Spoločný projekt DS-2016-0009, Relativistic effects in molecular materials based on gold complexes: catalytic activity, proton transfer, and NMR properties
- Technická univerzita v Berlíne, Nemecko (15.6. – 8.7.2017) Spolupráca v rámci APVV-15-0726 Rel-NMR-EPR - Vývoj nových teoretických nástrojov pre predikciu a interpretáciu EPR a NMR parametrov

Vladimír Malkin

- Paris-Lodron Universität Salzburg (7. – 11.9.2017) Spoločný projekt DS-2016-0009, Relativistic effects in molecular materials based on gold complexes: catalytic activity, proton transfer, and NMR properties
- Technická univerzita v Berlíne, Nemecko (15.6. – 8.7.2017) Spolupráca v rámci APVV-15-0726 Rel-NMR-EPR - Vývoj nových teoretických nástrojov pre predikciu a interpretáciu EPR a NMR parametrov

Helena Pálková

- Jerzy Haber Institute of Catalysis and Surface Chemistry PAS, Krakow, Poľsko (15. – 25. 10. 2017). Experimentálne práce v rámci spoločného projektu „Immobilization of metal nanoparticles on organo-modified layered silicates”. Medziakademická spolupráca (MAD) medzi Ústavom anorganickej chémie SAV a ústavom PAV.

Niketani Patel

- Research School of Engineering, College of Engineering & Computer Sciences, Australian National University, Canberra, Australia (1.12.2016-13.1.2017). Výskumný pobyt realizovaný v rámci

projektu SASPRO - Vlastnosti materiálov po vysokoteplotných koróziách v roztopených soliach.

Dlhodobé pobyty na zahraničných inštitúciách (viac ako 3 mesiace)

Marián Matejdes

- Yamaguchi University, Japonsko, 08/06/2015-07/06/2017, JSPS Fellowship Programs for Overseas Researches, ID No. P15742, JSPS KAKENHI Grant Number JP15F15742 (financovanie projektu).
Názov projektu: Photofunctionalities of nanosheets and nanosheet based materials: tuning their optical properties. Projekt sa zaoberá štúdiom a syntézou hybridných materiálov s prepínacími optickými vlastnosťami.

Peter Boháč

- Karlsruhe Institute of Technology. Nemecko, Sandwich VP project, 01/11/2017 - 06/06/2019.
Projekt sa zaoberá štúdiom bariér pre podzemné úložiská rádioaktívneho odpadu.

Prednášky zahraničných hostí na ÚACH SAV v roku 2017

Zhongning SHI (Northeastern University (NEU), Shenyang, Čína)

- Researches on molten salts chemistry and technology in Northeastern University (NEU), Shenyang, China, 28.9.2017
- Application of Fluoride Ionic liquids for Metals and Conducting Polymer Preparation, 28.9.2017

Xianwei HU (Northeastern University (NEU), Shenyang, Čína)

- Structural characterization of NaF-AlF₃-(CaF₂and/or BaF₂) melts in refined aluminum electrolysis by high temperature Raman spectroscopy

Xiaoli Tan, Ph. D (University of Alberta, Edmonton, Kanada)

- Roles of Fine solids/Clays in Water Based Bitumen Extraction from Alberta Oil Sands, 12.09.2017

prof. Makoto Hasegawa (Yokohama University, Japonsko)

- Delamination toughness in air plasma sprayed thermal barrier coatings, 19.7.2017

prof. Jingyang Wang (Chinese Academy of Sciences, Shenyang, Čína)

- High-throughput screening of rare earth silicates as environmental/thermal barrier coating and interfacial phase for SiCf/SiC CMCs, 7.7.2017

prof. Masahiro Yoshimura (National Cheng Kung University, Taiwan)

- Powder-less processing of nano-structured ceramics: possible direct fabrication of various advanced ceramics from solution and/or melt, 14.7.2017

Prof. Young-Wook Kim (Functional Ceramics Laboratory, Department of Mater. Sci. and Engineering, University of Seoul, Korea)

- Influence of grain growth on the electrical conductivity of liquid phase sintered SiC, 05.04.2017
- Factors affecting the thermal conductivity of liquid phase sintered SiC, 11.04.2017

*Prehľad údajov o medzinárodnej mobilite pracovníkov organizácie je uvedený v Prílohe E.
Prehľad a údaje o medzinárodných projektoch sú uvedené v kapitole 2 a Prílohe B.*

5. Vedná politika

Vedná politika ústavu reflektuje dlhodobé zámery a aktuálne trendy súvisiace so spoločenskou objednávkou na domácej a zahraničnej scéne. Je založená na inovatívnosti vedeckého smerovania, ambicióznosti vedeckých osobností, ako aj na autonómnosti vedúcich vedeckých tímov. Správnosť tohto smerovania dokumentuje pozícia ústavu, ktorý je hodnotený na popredných priečkach vo všetkých procesoch hodnotenia v SAV.

Základnými a dominantnými cieľmi, ktorým sú podriadené všetky aspekty chodu ústavu, sú odborný rast, medzinárodná integrácia a spoločenské uplatnenie/úžitok výsledkov výskumu. Napĺňanie uvedených cieľov si vyžaduje komplexný prienik aspektov, ako sú:

- aktívna účasť na domácich a zahraničných projektoch,
- aktívna publikačná činnosť v medzinárodných časopisoch a prezentácia výsledkov výskumu na medzinárodných vedeckých fórach,
- zachovanie vekovej a odbornej kontinuity,
- vytvorenie podmienok pre vzdelávanie a odborný rast nielen PhD študentov a mladých vedeckých pracovníkov, ale aj erudovaných vedeckých pracovníkov,
- aktívna účasť na vzdelávacom procese s dôrazom na druhý a tretí stupeň vysokoškolského vzdelania,
- technické zabezpečenie pre výskum,
- finančné zabezpečenie výskumu,
- personálna politika,
- zabezpečenie kontinuity v oblasti vedenia organizačných štruktúr ústavu, vytvorenie podmienok pre manažérsky rast pracovníkov,
- diseminácia a popularizácia objektov a výsledkov výskumu v odbornej a laickej spoločnosti,
- spolupráca a kooperácia s domácimi a zahraničnými akademickými, ako aj priemyselnými partnermi,
- zabezpečenie fungovania administratívnych požiadaviek.

Projektové tímy

Štruktúra ústavu v sebe inherentne zahŕňa flexibilné projektové tímy, ktoré sú vytvárané s ohľadom na objektové, resp. metodické možnosti a schopnosti jednotlivcov spájajúcich sa účelovo pri príprave a riešení projektov MŠ SR (štátne programy, projekty ŠF), VEGA, APVV, rámcových programov EÚ, NATO a v spolupráci s domácimi a zahraničnými partnermi z priemyslu. Táto flexibilná projektová štruktúra umožňuje pracovníkom resp. odborným skupinám podieľať sa na príprave vnútro-ústavných alebo aj mimo-ústavných vedeckých zoskupení, buď v rámci ústavu a SAV alebo aj mimo nich. Vedúci projektových tímov sú autonómni v rozhodovaní o spôsoboch riešenia projektu ako aj v nakladaní s finančnými prostriedkami v súlade s projektovými cieľmi a zmluvami.

Personálna politika

V oblasti personálnej politiky sa ústavu dlhodobo darí udržať relatívne nízky priemerný vek zamestnancov pod 47 rokov. Podpora zamestnávania mladých vedeckých pracovníkov patrí medzi prioritné úlohy vedenia ústavu. Pre zvýšenie počtu a motivácie mladých absolventov doktorandského štúdia, aby neodchádzali z oblasti vedy do finančne lukratívnejších zamestnaní, boli prijaté nasledujúce zásady personálnej politiky:

- Získavanie najlepších študentov na doktorandské štúdium vo vedných odboroch, ktoré má ústav akreditované ako externá vzdelávacia inštitúcia.
- Získavanie zahraničných doktorandov prostredníctvom projektov Marie Curie Research Training Network alebo iných schém podpory zahraničných študentov (napr. DAAD), v ktorých je ústav zapojený.
- Vysielanie čerstvých absolventov doktorandského štúdia na dlhodobé (najmenej 3 mesiace) pobyty do zahraničia, aby sa zoznámili s najmodernejšou prístrojovou technikou, laboratórnymi postupmi a metódami práce vo vyspelých pracoviskách v Európe a vo svete (najčastejšie Japonsko a USA).
- Organizovanie medzinárodných podujatí doma, ako aj vysielanie mladých vedeckých pracovníkov a doktorandov na renomované konferencie v zahraničí s cieľom získať skúsenosti s prezentovaním

vedeckých výsledkov.

- Pozývanie renomovaných odborníkov zo zahraničia na prednášky pre doktorandov a zamestnancov ústavu.

S cieľom plnenia stanovených zásad personálnej politiky sa Ústav anorganickej chémie ako hostiteľská organizácia pridal k úspešným prijímateľom projektov mobilného programu Slovenskej akadémie vied – SASPRO – aktuálne traja štipendisti.

Technická infraštruktúra

Neoddeliteľnou súčasťou vednej politiky je aj rozvoj infraštruktúry. Ústav cielene buduje svoju infraštruktúru na rôznych úrovniach cez laboratóriá na prípravu vzoriek až po laboratória na charakterizáciu pripravených materiálov. Vyžaduje si to dlhodobú aktivitu postupnej rekonštrukcie priestorov, ktorá je pre svoje špecifické požiadavky náročná ako finančne, tak aj časovo, pretože prebieha pri plnej prevádzke ostatných zariadení. Prístrojové vybavenie sleduje vzájomnú komplementaritu techník. Snahou je aj poskytovať voľné časové kapacity na merania pre partnerov na Slovensku, ako aj zapájanie ústavu prostredníctvom technickej infraštruktúry do medzinárodných zväzkov.

6. Spolupráca s univerzitami/vysokými školami, štátnymi a neziskovými inštitúciami okrem aktivít uvedených v kap. 2, 3, 4

6.1. Spolupráca s univerzitami/VŠ (fakultami)

Názov univerzity/vysokej školy a fakulty: Prírodovedecká fakulta UK

Druh spolupráce (spoločné pracovisko alebo iné): Spoločná výchova doktorandov, spoločné riešenie projektov, spolupráca v pedagogickom procese

Začiatok spolupráce: 1990

Zameranie: vedecká spolupráca, účasť na Bc. a Mgr. výuke

Zhodnotenie: V spolupráci s touto fakultou je ústav zapojený do vzdelávania na III. stupni vysokoškolského štúdia v študijných programoch anorganická chémia a chemická fyzika. Spoločne sa riešia projekty VEGA a APVV. Prof. RNDr. J. Noga, DrSc. a doc. RNDr. J. Bujdák, DrSc. majú hlavný úväzok na fakulte a čiastkový na ÚACH SAV. Prof. RNDr. J. Noga, DrSc. je externým členom Vedeckej rady ÚACH SAV. Pracovníci ÚACH viedli na PríF UK v roku 2017 dvoch doktorandov.

Názov univerzity/vysokej školy a fakulty: Fakulta chemickej a potravinárskej technológie STU

Druh spolupráce (spoločné pracovisko alebo iné): Spoločné pracovisko, spoločná výchova doktorandov

Začiatok spolupráce: 1990

Zameranie: vedecká spolupráca

Zhodnotenie: Na základe dodatku k zmluve o zriadení spoločného pracoviska je FCHPT od roku 2008 členom konzorcia a spoluzriaďovateľom spoločného pracoviska, Centra kompetencie skla Vitrum Laugaricio – VILA. Pracovníci ÚACH viedli na FCHPT v roku 2017 piatich doktorandov (z toho dvaja externí).

Názov univerzity/vysokej školy a fakulty: Fakulta materiálov, metalurgie a recyklácie TUKE

Druh spolupráce (spoločné pracovisko alebo iné): Spolupráca v pedagogickom procese

Začiatok spolupráce: 2000

Zameranie: vedecká spolupráca, účasť na Bc. a Mgr. výuke

Zhodnotenie: V spolupráci s touto fakultou je ústav zapojený do pedagogického procesu. Prof. RNDr. P. Šajgalík, DrSc. je členom vedeckej rady fakulty.

Názov univerzity/vysokej školy a fakulty: Trenčianska univerzita Alexandra Dubčeka v Trenčíne

Druh spolupráce (spoločné pracovisko alebo iné): Centrum kompetencie skla - Vitrum Laugaritio

Začiatok spolupráce: 1997

Zameranie: vedecká spolupráca

Zhodnotenie: Okrem spoločného pracoviska s TnU AD (Centrum kompetencie skla Vitrum Laugaritio) riešil ÚACH SAV v roku 2016 v spolupráci s touto univerzitou jeden spoločný projekt VEGA a dva spoločné projekty APVV. Prof. Ing. P. Galusek, DrSc. prorektor pre vedu, výskum a medzinárodné vzťahy TnU AD je aj členom Vedeckej rady TnU AD a dvoch jej fakúlt (Fakulty zdravotníctva a Fakulty špeciálnej techniky), prof. Ing. M. Liška, DrSc. je externým členom Vedeckej rady ÚACH. Pracovníci centra, zamestnanci ÚACH, sa podieľajú na pedagogickej činnosti v rámci vysokoškolského štúdia v odbore "Chemické technológie" a doktorandského štúdia v odbore "Anorganická technológia".

Názov univerzity/vysokej školy a fakulty: Vysoká škola báňská - TU Ostrava, Česká republika

Druh spolupráce (spoločné pracovisko alebo iné): Spoločná výchova doktorandov, spoločné riešenie projektov

Začiatok spolupráce: 2010

Zameranie: vedecká spolupráca, výchova doktorandov

Zhodnotenie: Spolupráca VŠB a ÚACH je zameraná na výchovu mladých pracovníkov. Na ÚACH pokračovala vo svojom štúdiu jedna doktorandka z VŠB Ostrava. Prof. RNDr. P. Šajgalík, DrSc. je členom Vedeckej rady FMFI VŠB; doc. Ing. Z. Lenčoš, PhD. je členom odborovej rady doktorandského študijného programu Materiálové vedy a inžinýrství.

Názov univerzity/vysokej školy a fakulty: University of Ghent, Belgicko

Druh spolupráce (spoločné pracovisko alebo iné): Department of Inorganic and Physical Chemistry

Začiatok spolupráce: 2010

Zameranie: vedecká spolupráca

Zhodnotenie: Vedecká spolupráca pri príprave amorfných a polykryštalických materiálov sol-gel metódami v systémoch $\text{Al}_2\text{O}_3\text{-La}_2\text{O}_3$, $\text{Al}_2\text{O}_3\text{-La}_2\text{O}_3\text{-ZrO}_2$, $\text{Al}_2\text{O}_3\text{-Y}_2\text{O}_3$. Skúmanie vlastností pripravených materiálov a spoločné publikácie.

6.2. Významné aplikácie výsledkov výskumu v spoločenskej praxi alebo vyriešenie problému pre štátnu alebo neziskovú inštitúciu

6.3. Iná činnosť využiteľná pre potreby spoločenskej praxe

7. Spolupráca s aplikačnou a hospodárskou sférou okrem aktivít uvedených v kap. 2, 3, 4

7.1. Spoločné pracoviská s aplikačnou sférou

Názov pracoviska: Spoločné pracovisko Ústavu anorganickej chémie Slovenskej akadémie vied a RONA, a.s.

Partner(i): Rona a.s., Lednické Rovne

Zameranie: Stimulácia, rozvoj a realizácia základného a aplikovaného výskumu a vývoja v oblastiach súvisiacich s existujúcou priemyselnou základňou SR

Rok založenia: 2011

Zhodnotenie: V roku 2016 RONA a.s. podala projekt v rámci výziev štrukturálnych fondov, v ktorom ústav vystupuje ako partner.

7.2. Kontraktový – zmluvný výskum (vrátane zahraničných kontraktov)

Názov kontraktu: Výskum a vývoj pokročilých žiaruvzdorných materiálov na báze Al-Si-O-C-N a Zr-O-C-N

Partner(i): RHI AG Leoben, Rakúsko

Začiatok spolupráce (v súlade s podpísaným kontraktom): 2017

Ukončenie spolupráce (ak ide o spoluprácu v krátkom období): trvá

Objem získaných prostriedkov v bežnom roku (€): 0

Stručný opis výstupu/výsledku: P. Šajgalík, Z. Lenčoš

Zhodnotenie:

Názov kontraktu: Vývoj transparentnej keramiky a iných materiálov

Partner(i): CEIT a.s.

Začiatok spolupráce (v súlade s podpísaným kontraktom): 2017

Ukončenie spolupráce (ak ide o spoluprácu v krátkom období): trvá

Objem získaných prostriedkov v bežnom roku (€): 0

Stručný opis výstupu/výsledku:

Zhodnotenie:

7.3. Iná činnosť využiteľná pre potreby hospodárskej praxe

Ústav disponuje kvalitnými odbornými personálnymi kapacitami ako aj kvalitným a moderným technickým vybavením, ktoré sú k dispozícii našim akademickým ale aj priemyselným partnerom. Práve títo priemyselní partneri sa obracajú na náš ústav s otázkami riešenia ich partikulárnych problémov. Na druhej strane aj ústav intenzívne vyhľadáva priemyselných partnerov doma ale aj v zahraničí. Týmto spôsobom sa ústav aktívne podieľa na riešení problémov hospodárskej praxe, popri svojej základnej úlohe základného výskumu.

8. Aktivity pre Národnú radu SR, vládu SR, ústredné orgány štátnej správy SR a iné organizácie

8.1. Členstvo v poradných zboroch vlády SR, Národnej rady SR, ministerstiev SR, orgánoch EÚ, EP, NATO a pod.

Tabuľka 8a Členstvo v poradných zboroch Národnej rady SR, vlády SR, ministerstiev SR, orgánoch EÚ, EP, NATO a pod.

Meno pracovníka	Názov orgánu	Funkcia
prof. Ing. Dušan Galusek, DrSc.	Slovenský metrologický ústav	člen vedeckej rady
Mgr. Stanislav Kedžuch, PhD.	Slovenská komisia chemickej olympiády	podpredseda
Ing. Michal Korenko, PhD.	Komisia pre námietky pri verejnom obstarávaní	externý člen
RNDr. Jana Madejová, DrSc.	Agentúra na podporu výskumu a vývoja	Člen rady pre prírodné vedy
prof. RNDr. Jozef Noga, DrSc.	Akreditačná komisia SR	člen pracovnej skupiny pre oblasť výskumu Chémia, chemická technológia a biotechnológie
prof. RNDr. Pavol Šajgalík, DrSc.	Komisia ministra školstva pre udeľovanie Ceny ministra školstva	člen
	Slovenská komisia pre vedecké hodnosti (SKVH)	podpredseda
	Výskumná agentúra SR	člen
	Technologická agentúra SR	člen
	Rada predsedov pracovných skupín pre prioritné oblasti aplikovaného výskumu a experimentálneho vývoja	predseda
	Komisia MŠ pre prioritné oblasti aplikovaného výskumu a experimentálneho vývoja v SR - materiálový výskum a nanotechnológie	člen pracovnej skupiny
	Pandemická komisia MZ SR	člen
	Rada vlády pre vedu, techniku a inovácie	podpredseda

8.2. Expertízna činnosť a iné služby pre štátnu správu a samosprávy

8.3. Členstvo v radách štátnych programov a podprogramov ŠPVV a ŠO

Tabuľka 8b Členstvo v radách štátnych programov a podprogramov ŠPVV a ŠO

Meno pracovníka	Názov orgánu	Funkcia
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8.4. Prehľad aktuálnych spoločenských problémov, ktoré riešilo pracovisko v spolupráci s Kanceláriou prezidenta SR, s vládnyimi a parlamentnými orgánmi alebo pre ich potrebu

9. Vedecko-organizačné a popularizačné aktivity

9.1. Vedecko-popularizačná činnosť

Tabuľka 9a Súhrnné počty vedecko-popularizačných činností organizácie SAV

Typ	Počet	Typ	Počet	Typ	Počet
prednášky/besedy	1	tlač	0	TV	1
rozhlas	0	internet	0	exkurzie	1
publikácie	0	multimediálne nosiče	0	dokumentárne filmy	0
iné	0				

9.2. Vedecko-organizačná činnosť

Tabuľka 9b Vedecko-organizačná činnosť

Názov podujatia	Domáca/ medzinárodná	Miesto	Dátum konania	Počet účastníkov
4. seminár Slovenskej ílovej spoločnosti - Ílové minerály a vybrané nerudné suroviny v materiálovom výskume, priemyselných aplikáciách a životnom prostredí	domáca	Kongresové centrum SAV, Hotel Academia	19.06.-21.06.2017	29
Aplikácie v UV-Vis-NIR spektrofotometrii	domáca	Bratislava	26.09.-27.09.2017	30
10th Workshop on Modern Methods in Quantum Chemistry	medzinárodná	Mariapfarr, Rakúsko	05.03.-10.03.2017	56

9.3. Účasť na výstavách

Názov výstavy: Európska Noc výskumníkov 2017

Miesto konania: Stará tržnica, Bratislava

Dátum: 29.9.2017

Zhodnotenie účasti: Prezentácia výskumu a výsledkov oddelenia keramiky, oddelenia hydrosilikátov a oddelenia taveninových sústav (R. Bystrický, M. Hičák, V. Bizovská, P. Boháč, M. Slaný, S. Belušáková, M. Kontrík, M. Barlog, Z. Fördösová, V. Pavlík). Stánok: SVET ANORGANICKÝCH MATERIÁLOV

9.4. Účasť v programových a organizačných výborych národných konferencií

Tabuľka 9c Programové a organizačné výbory národných konferencií

Meno pracovníka	Programový	Organizačný	Programový i organizačný
Madejová Jana	0	0	1
Pálková Helena	0	1	0
Spolu	0	1	1

9.5. Členstvo v redakčných radách časopisov

doc. Ing. Miroslav Boča, DrSc.

Chemical Papers (funkcia: Editorial Advisory Board od 9/2013)

doc. RNDr. Juraj Bujdák, DrSc.

Applied Clay Science (funkcia: associate editor)

Chemistry Africa (Springer) (funkcia: associate editor)

ChemistrySelect (Wiley-VCH) (funkcia: člen redakčnej rady)

prof. Ing. Dušan Galusek, DrSc.

Ceramics-Silikáty (funkcia: člen)

New Journal of Glass and Ceramics (funkcia: člen)

RNDr. Peter Komadel, DrSc.

Applied Clay Science (funkcia: člen)

Clay Minerals (funkcia: člen)

Geologica Carpathica (funkcia: člen)

doc. Ing. Zoltán Lenčič, PhD.

Journal of the Ceramic Society of Japan (funkcia: člen)

prof. Ing. Marek Liška, DrSc.

Ceramics - Silikáty (funkcia: člen)

European Journal of Glass Science and Technology (funkcia: regional editor)

International Journal of Applied Glass Science (funkcia: člen)

Sklár a keramik (funkcia: člen)

RNDr. Jana Madejová, DrSc.

Clays and Clay Minerals (funkcia: associate editor)

prof. RNDr. Pavol Šajgalík, DrSc.

Ceramics-Silikáty (funkcia: člen)

Journal of Asian Ceramic Society (funkcia: spolueditor)

Journal of Ceramic Science and Technology (funkcia: člen)

Keramický Zpravodaj (funkcia: člen)

Processing and Application of Ceramics (funkcia: člen)

9.6. Činnosť v domácich vedeckých spoločnostiachMgr. Silvia Belušáková, PhD.

Slovenská ílová spoločnosť (funkcia: člen)

Mgr. Valéria Bizovská, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská ílová spoločnosť (funkcia: člen)

doc. Ing. Miroslav Boča, DrSc.

Humboldtov klub v SR (funkcia: člen)

Slovenská chemická spoločnosť (funkcia: člen)

Mgr. Peter Boháč, PhD.

Slovenská ílová spoločnosť (funkcia: člen)

doc. RNDr. Juraj Bujdák, DrSc.

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská ílová spoločnosť (funkcia: člen výboru)

Mgr. Roman Bystrický, PhD.

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)

Mgr. Adriana Czímerová, PhD.

Slovenská ílová spoločnosť (funkcia: člen)

Mgr. Alexander Čeklovský, PhD.

Slovenská spektroskopická spoločnosť (funkcia: člen)

prof. Ing. Dušan Galusek, DrSc.

Humboldtov klub v SR (funkcia: člen)

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)

Slovenská sklárska spoločnosť (funkcia: člen predstavenstva, vedecký tajomník)

Ing. Veronika Gurišová

Slovenská chemická spoločnosť (funkcia: člen)

Ing. Ondrej Hanzel, PhD.

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)

doc. Ing. Miroslav Hnatko, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)

Ing. Mária Chromčíková, PhD.

Česká sklárska spoločnosť (funkcia: člen)

Slovenská sklárska spoločnosť (funkcia: člen)

Mgr. Ľuboš Jankovič, PhD.

Slovenská ílová spoločnosť (funkcia: člen)

Mgr. Stanislav Kedžuch, PhD.

Slovenská chemická spoločnosť (funkcia: člen predsedníctva)

RNDr. Peter Komadel, DrSc.

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská ílová spoločnosť (funkcia: člen)

Učená spoločnosť SAV (funkcia: člen)

Ing. Michal Korenko, PhD.

Slovenská chemická spoločnosť (funkcia: predseda revíznej komisie)

Slovenská nukleárna spoločnosť (funkcia: člen)

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)

Slovenská spoločnosť pre povrchové úpravy (funkcia: člen)

Ing. Blanka Kubíková, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

doc. Ing. Zoltán Lenčéš, PhD.

Humboldtov klub v SR (funkcia: člen)

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen výboru)

prof. Ing. Marek Liška, DrSc.

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská sklárska spoločnosť (funkcia: člen)

RNDr. Jana Madejová, DrSc.

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská ílová spoločnosť (funkcia: podpredseda)

Učená spoločnosť SAV (funkcia: člen)

Ing. Jarmila Mlynáriková, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

Ing. Zuzana Netriová, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

prof. RNDr. Jozef Noga, DrSc.

Humboldtov klub v SR (funkcia: člen)

Slovenská akademická spoločnosť (funkcia: podpredseda)

Učená spoločnosť SAV (funkcia: predseda)

Ing. Helena Pálková, PhD.

Slovenská ílová spoločnosť (funkcia: člen výboru)

Ing. Viliam Pavlík, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

Mgr. Lukáš Petra

Slovenská ílová spoločnosť (funkcia: člen)

Ing. Anna Prnová, PhD.

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)

Slovenská Sklárska spoločnosť (funkcia: člen)

Ing. Jaroslav Sedláček, PhD.

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)

Ing. Eva Scholtzová, CSc.

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská ílová spoločnosť (funkcia: člen)

Ing. Michal Slaný

Slovenská ílová spoločnosť (funkcia: člen)

prof. RNDr. Pavol Šajgalík, DrSc.

Humboldtov klub v SR (funkcia: člen)

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská silikátová vedecko-technická spoločnosť (funkcia: predseda)

Slovenská sklárska spoločnosť (funkcia: člen predstavenstva)

Učená spoločnosť SAV (funkcia: člen)

Ing. František Šimko, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

doc. Ing. Peter Šimurka, PhD.

Slovenská sklárska spoločnosť (funkcia: predseda)

Zväz slovenských vedecko-technických spoločností (funkcia: člen rady)

Mgr. Peter Švančárek, PhD.

Slovenská sklárska spoločnosť (funkcia: člen)

Ing. Zuzana Vasková, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

9.7. Iné dôležité informácie o vedecko-organizačných a popularizačných aktivitách

Dňa 07.11.2017 už tradične zorganizoval Ústav anorganickej chémie SAV v rámci Týždňa vedy a techniky na Slovensku „Deň otvorených dverí ÚACH SAV“, na ktorý boli pozvaní študenti stredných ako aj vysokých škôl zo Slovenska. Pre mladých návštevníkov boli pripravené zaujímavé prednášky „Svet moderných keramických materiálov“ ako aj „Veda a výskum na ÚACH“. Prehliadka ústavu pre študentov

potom pokračovala na stanovištiach (Stlačené peklo..., Ľadová romantika..., Tajomstvá chémie..., Elektrónová strelba na živé organizmy..., Íl, ktorý nie je iba hlina..., Čiarové kódy prírody..., Inteligentné vibrácie...) vo vybraných laboratóriách, pričom mladí vedeckí pracovníci ukazovali prístroje ktoré používajú pri analýze materiálov, žiarové lisy, vymrazovací granulátor a podobne. Záujemcov informovali o praktickom využití zariadení, prípadne im názorne aj ich využitie prezentovali. Na niektorých stanovištiach im zároveň predviedli efektné a zaujímavé chemické experimenty. Návštevníkov zaujala prezentácia pripravená na skenovanom elektrónovom mikroskope, chemické experimenty a rôzne pokusy s tekutým dusíkom. Dňa otvorených dverí sa zúčastnilo približne 190 študentov z bratislavských aj mimobratislavských stredných škôl (Trnava, Liptovský Mikuláš).

10. Činnosť knižnično-informačného pracoviska

10.1. Knižničný fond

Tabuľka 10a Knižničný fond

Knižničné jednotky spolu		7582
z toho	knihy a zviazané periodiká	7582
	audiovizuálne dokumenty	
	elektronické dokumenty (vrátane digitálnych)	
	mikroformy	
	iné špeciálne dokumenty - dizertácie, výskumné správy	
	Rukopisy, vzácne tlače	
Počet titulov dochádzajúcich periodík		
z toho zahraničné periodiká		
Ročný prírastok knižničných jednotiek		10
v tom	kúpou	10
	darom	
	výmenou	
	bezodplatným prevodom	
	náhradou	
Úbytky knižničných jednotiek		
Knižničné jednotky spracované automatizovane		

Výraz „**v tom**“ označuje úplné (vyčerpávajúce) údaje, ktorých súčet sa musí rovnať údaju v riadku „spolu“, čiže nadradenému riadku.

Výraz „**z toho**“ označuje neúplné (výberové) údaje, ktorých súčet sa nemusí rovnať údaju v riadku „spolu“.

10.2. Výpožičky a služby

Tabuľka 10b Výpožičky a služby

Výpožičky spolu (riadok 1)		58
v tom z r. 1	prezenčné výpožičky	8
	absenčné výpožičky	
v tom z r. 1	odborná literatúra pre dospelých	28
	výpožičky periodík	22
MVS iným knižniciam		
MVS z iných knižníc		
MMVS iným knižniciam		
MMVS z iných knižníc		
Počet vypracovaných bibliografií		
Počet vypracovaných rešerší		

10.3. Používatelia

Tabuľka 10c Používatelia

Registrovaní používatelia	60
Návštevníci knižnice spolu (bez návštevníkov podujatí)	65

10.4. Iné údaje**Tabuľka 10d Iné údaje**

On-line katalóg knižnice na internete (1=áno, 0=nie)	
Náklady na nákup knižničného fondu v €	462,58

10.5. Iné informácie o knižničnej činnosti

11. Aktivity v orgánoch SAV

11.1. Členstvo vo Výbore Snemu SAV

11.2. Členstvo v Predsedníctve SAV a vo Vedeckej rade SAV

prof. RNDr. Pavol Šajgalík, DrSc.

- Predseda SAV
- predseda VR SAV

11.3. Členstvo vo vedeckých kolégiách SAV

doc. Ing. Miroslav Boča, DrSc.

- VK SAV pre chemické vedy (člen)

RNDr. Peter Komadel, DrSc.

- VK SAV pre chemické vedy (člen)

RNDr. Jana Madejová, DrSc.

- VK SAV pre chemické vedy (člen)

prof. RNDr. Jozef Noga, DrSc.

- VK SAV pre chemické vedy (člen)

prof. RNDr. Pavol Šajgalík, DrSc.

- VK SAV pre chemické vedy (člen)

11.4. Členstvo v komisiách SAV

doc. Ing. Miroslav Boča, DrSc.

- Komisia SAV pre vyhodnocovanie medzinárodných projektov (člen)

RNDr. Peter Komadel, DrSc.

- Komisia SAV pre zahraničné styky (člen)

11.5. Členstvo v orgánoch VEGA

doc. Ing. Miroslav Boča, DrSc.

- Komisia VEGA č. 3 pre chemické vedy, chemické inžinierstvo a biotechnológie (predseda)

RNDr. Peter Komadel, DrSc.

- Komisia VEGA č. 3 pre chemické vedy, chemické inžinierstvo a biotechnológie (člen)

doc. Ing. Zoltán Lenčoš, PhD.

- Komisia VEGA č. 7 pre strojárstvo a príbuzné odbory informačných a komunikačných technológií a materiálové inžinierstvo (člen)

Dr. Oľga Malkin, DrSc.

- Komisia VEGA č. 3 pre chemické vedy, chemické inžinierstvo a biotechnológie (člen)

12. Hospodárenie organizácie

12.1. Výdavky RO SAV

Tabuľka 12a Výdavky RO SAV (v €)

V ý d a v k y	Skutočnosť k 31.12.2017 spolu	v tom:		
		zo ŠR	z toho: ŠF EÚ vr. spolufinan .zo ŠR	z mimorozp. zdrojov
				z toho: ŠF EÚ vr. spolufinan.zo ŠR
Výdavky spolu	2 010 788	1 427 280		583 508
Bežné výdavky	1 974 341	1 405 456		58 905
v tom:				
mzdy (610)	940 999	812 793		9 493
poistné a príspevok do poisťovní (620)	325 973	288 366		524
tovary a služby (630)	548 889	269 656		48 888
z toho: časopisy	1 455	1 399		
VEGA projekty	107 600	107 600		
MVTS projekty	41 273	41 273		
CE				
vedecká výchova	1 760	1 760		
bežné transfery (640)	34 641	34 641		
z toho: štipendiá	29 401	29 401		
transfery partnerom projektov	123 839			123 839
Kapitálové výdavky	36 447	21 824		12 960
v tom:				
obstarávanie kapitálových aktív	36 447	21 824		12 960
kapitálové transfery				
z toho: transfery partnerom projektov				

12.2. Príjmy RO SAV

Tabuľka 12b Príjmy RO SAV (v €)

P r í j m y	Skutočnosť k 31.12.2017 spolu	v tom:	
		rozpočtové	z mimorozp. zdrojov
Príjmy spolu	602 075	18 567	583 508
Nedaňové príjmy	602 075	18 567	583 508
v tom:			
príjmy z prenájmu	1 671	1 671	
príjmy z predaja výrobkov a služieb	16 896	16 896	
iné	583 508		583 508
Granty a transfery (mimo zdroja 111)	583 508		583 508
v tom:			
tuzemské	572 935		572 935
z toho: APVV	483 428		483 428
iné	89 507		89 507
zahraničné	10 573		10 573
z toho: projekty rámcového programu EÚ			
iné	10 573		10 573

13. Nadácie a fondy pri organizácii SAV

14. Iné významné činnosti organizácie SAV

15. Vyznamenania, ocenenia a ceny udelené pracovníkom organizácie v roku 2017

15.1. Domáce ocenenia

15.1.1. Ocenenia SAV

Maďejová Jana

Ocenenia pre najúspešnejších autorov SAV

Oceňovateľ: Predsedníctvo SAV

Opis: Vysoko citované publikácie s najvyšším počtom citácií získaných v priebehu rokov 2013 – 2015, ktoré zároveň podľa parametrov databázy Essential Science Indicators Web of Science patria medzi tzv. Highly Cited Papers. Počty citácií sú normované na priemernú citovanosť v danom vednom odbore.

MADEJOVÁ, J. FTIR techniques in clay mineral studies. In Vibrational Spectroscopy, 2003, vol. 31, p. 1-10 (spolu 682 citácií)

Noga Jozef

Ocenenia pre najúspešnejších autorov SAV

Oceňovateľ: Predsedníctvo SAV

Opis: Vysoko citované publikácie s najvyšším počtom citácií získaných v priebehu rokov 2013 – 2015, ktoré zároveň podľa parametrov databázy Essential Science Indicators Web of Science patria medzi tzv. Highly Cited Papers. Počty citácií sú normované na priemernú citovanosť v danom vednom odbore.

HELGAKE, 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 (spolu 1386 citácií)

15.1.2. Iné domáce ocenenia

15.2. Medzinárodné ocenenia

16. Poskytovanie informácií v súlade so zákonom č. 211/2000 Z. z. o slobodnom prístupe k informáciám v znení neskorších predpisov (Zákon o slobode informácií)

17. Problémy a podnety pre činnosť SAV

Zásadný problém, ktorý narastá niekoľko rokov a v roku 2017 sa prejavil bez náznakov zlepšenia, je absurdný nárast administratívnych nárokov na všetkých úrovniach. Dominuje im oblasť verejného obstarávania. Pre potreby naplnenia legislatívnych povinností ústavu v oblasti verejného obstarávania je jeden plný úväzok pre administratívneho pracovníka málo, ale mzdové prostriedky ústavu neumožňujú rozšírenie administratívy. Výsledkom je, že potrebnú aktivitu vykonáva približne 5 vedeckých pracovníkov nad rámec alebo na úkor svojich odborných aktivít. Táto situácia je absolútne neúnosná. Deklarovaná snaha P SAV pomôcť ústavom v tejto situácii je vítaná, ale stále nie je naplnená.

Iným príkladom absurdnej administratívnej povinnosti je sledovanie výdavkov na nákup výpočtovej techniky v samostatnej kapitole. Výsledkom je požiadavka presne definovať sumu vyčlenenú na túto aktivitu s tým, že akékoľvek schvalovanie trvá 2-3 mesiace! To znamená, že posledný nákup z projektov môže byť realizovaný možno v septembri aby sa stihol celý schvalovací proces.

Jednou z možností, ako by mohlo Predsedníctvo pomôcť ústavom s prebujnelou administratívou, je zabezpečiť poistenie majetku (hlavne z dôvodu požiadavky VA) pre všetky ústavy centrálnе, čo by ústavy výrazne odbremenilo a pravdepodobne by sa podarilo vyrokovať nižšie ceny na poistné zmluvy od jedného dodávateľa pre väčšie množstvo prístrojov. Okrem toho chýbajú z pozície P SAV aj ďalšie aktivity v rovine všeobecných usmernení, napr. usmernenia a prípadne školenia ako postupovať pri aplikácií elektronického trhoviska.

Proces transformácie SAV bol síce naštartovaný ale intenzita komunikácie v tejto otázke nie je dostatočná, je viac menej sporadická a pomerne komplikovaná. V tejto komunikácii sa navyše riešia iba otázky, ktoré pre P SAV vyplývajú zo zákona a výsledkom je, že každý ústav bude musieť vypracovať množstvo dokumentov toho istého typu samostatne. Preto by sme uvítali podporu P SAV aj v tomto smere.

Ďalším problémom presahujúcim možnosti riešenia jednotlivého ústavu, je prístup agentúry APVV k otázke čerpania nepriamych nákladov. Tento prístup zásadným spôsobom obmedzuje fungovanie organizácie, pričom jednostranná interpretácia zákona zo strany APVV nie je konfrontovaná iným nezávislým zdrojom.

Správu o činnosti organizácie SAV spracoval(i):

doc. Ing. Zoltán Lenčéš, PhD., 02/59410408

Ing. Helena Pálková, PhD., 02/59410485

Riaditeľ organizácie SAV

Predseda vedeckej rady

.....
doc. Ing. Miroslav Boča, DrSc.

.....
RNDr. Jana Madejová, DrSc.

Prílohy**Príloha A - Zoznam zamestnancov a doktorandov organizácie k 31.12.2017****Zoznam zamestnancov podľa štruktúry (nadväzne na údaje v Tabuľke 1a)**

	Meno s titulmi	Úväzok (v %)	Ročný prepočítaný úväzok
Vedúci vedeckí pracovníci DrSc.			
1.	doc. Ing. Miroslav Boča, DrSc.	100	1.00
2.	doc. RNDr. Juraj Bujdák, DrSc.	50	0.50
3.	prof. Ing. Dušan Galusek, DrSc.	55	0.55
4.	RNDr. Peter Komadel, DrSc.	100	1.00
5.	prof. Ing. Marek Liška, DrSc.	45	0.45
6.	RNDr. Jana Madejová, DrSc.	100	1.00
7.	Dr. Oľga Malkin, DrSc.	100	1.00
8.	Dr. Vladimír Malkin, DrSc.	100	1.00
9.	prof. RNDr. Jozef Noga, DrSc.	53	0.53
10.	prof. RNDr. Pavol Šajgalík, DrSc.	55	0.55
Samostatní vedeckí pracovníci			
1.	doc. Ing. Tomáš Bučko, PhD.	25	0.25
2.	Mgr. Adriana Czímerová, PhD.	100	1.00
3.	doc. Ing. Miroslav Hnatko, PhD.	100	1.00
4.	Ing. Mária Chromčíková, PhD.	100	1.00
5.	Mgr. Ľuboš Jankovič, PhD.	100	1.00
6.	Mgr. Stanislav Kedžuch, PhD.	100	1.00
7.	Mgr. Stanislav Komorovský, PhD.	100	1.00
8.	Ing. Michal Korenko, PhD.	100	1.00
9.	Ing. Blanka Kubíková, PhD.	100	1.00
10.	doc. Ing. Zoltán Lenčéš, PhD.	100	1.00
11.	Ing. Helena Pálková, PhD.	100	1.00
12.	Ing. Viliam Pavlík, PhD.	100	1.00
13.	Ing. Anna Prnová, PhD.	100	1.00
14.	Ing. Jaroslav Sedláček, PhD.	100	1.00
15.	Ing. Eva Scholtzová, CSc.	100	1.00
16.	Ing. František Šimko, PhD.	100	1.00
17.	doc. Ing. Peter Šimurka, PhD.	100	0.40

18.	Mgr. Peter Švančárek, PhD.	100	1.00
19.	Ing Peter Tatarko, PhD.	100	1.00
20.	Ing. Štefan Varga, CSc.	100	1.00
Vedeckí pracovníci			
1.	James Richard Asher, PhD	100	1.00
2.	Mgr. Silvia Belušáková, PhD.	100	0.33
3.	Mgr Valéria Bizovská, PhD.	100	1.00
4.	Mgr. Peter Boháč, PhD.	100	1.00
5.	Mgr. Roman Bystrický, PhD.	120	1.20
6.	Mgr. Alexander Čeklovský, PhD.	100	1.00
7.	Ing. Ondrej Hanzel, PhD.	100	1.00
8.	Ing. Martin Kontrík, PhD.	100	1.00
9.	Ing. Monika Micháľková, PhD.	70	0.00
10.	Ing. Jarmila Mlynáriková, PhD.	100	1.00
11.	Ing. Zuzana Netriová, PhD.	100	1.00
12.	Dr. Niketan Patel Sarabhai	100	1.00
13.	Dr. Mohamed Radwan	100	1.00
14.	Ing. Peter Škorňa, PhD.	100	0.33
15.	Ing. Jana Valúchová, PhD.	100	1.00
16.	Ing. Zuzana Vasková, PhD.	100	0.00
Odborní pracovníci s VŠ vzdelaním (výskumní a vývojoví zamestnanci)			
1.	Ing. Veronika Gurišová	100	0.00
2.	Ing. Eva Hadzimová	100	0.00
3.	Ing. Iveta Macková	100	1.00
4.	Ing. Eva Mikšíková	125	1.25
5.	Ing. Jozef Priščák	100	1.00
6.	Mgr. Pavol Weiner	100	1.00
Odborní pracovníci s VŠ vzdelaním (ostatní zamestnanci)			
1.	Rastislav Haška	100	1.00
2.	Ing. Ingrid Hierwegová	5	0.05
3.	Ing. Ján Piško	100	1.00
4.	Ing. Jaroslav Rusnák, PhD.	33	0.33
5.	JUDr. Bc. Marica Slaná	100	1.00
6.	JUDr. Jana Šebová	100	1.00
Odborní pracovníci ÚSV			

1.	Miroslav Baďura	20	0.20
2.	Iveta Bouadjenak	100	1.00
3.	Jaromíra Dankovičová	125	1.25
4.	Jarmila Heinleinová	100	1.00
5.	Miriám Hnatková	100	0.00
6.	Anna Jurová	100	1.00
7.	Magdaléna Kňazovičová	100	0.50
8.	Anna Kovárová	100	1.00
9.	Zora Lukáčová	100	1.00
10.	Jozef Sitár	100	1.00
11.	Mária Strempekova	100	1.00
12.	Alexandra Tonkovičová	100	1.00
Ostatní pracovníci			
1.	Margita Hudáková	100	1.00
2.	Terézia Pírová	100	1.00

Zoznam zamestnancov, ktorí odišli v priebehu roka

	Meno s titulmi	Dátum odchodu	Ročný prepočítaný úväzok
Samostatní vedeckí pracovníci			
1.	doc. Ing. Peter Šimurka, PhD.	31.12.2017	0.40
Vedeckí pracovníci			
1.	Mgr Marián Matejdes, PhD.	7.6.2017	0.00
Odborní pracovníci s VŠ vzdelaním (výskumní a vývojoví zamestnanci)			
1.	Ing. Veronika Gurišová	31.12.2017	0.00
Odborní pracovníci s VŠ vzdelaním (ostatní zamestnanci)			
1.	Ing. Irena Martel	30.6.2017	0.50
Ostatní pracovníci			
1.	Dana Matejkinová	31.5.2017	0.00

Zoznam doktorandov

	Meno s titulmi	Škola/fakulta	Študijný odbor
Interní doktorandi hrazení z prostriedkov SAV			
1.	Ing. Martin Barlog	Slovenská technická univerzita v Bratislave	5.2.19 anorganická technológia a materiály
2.	Ing. Zuzana Fördösová	Slovenská technická univerzita v Bratislave	5.2.19 anorganická technológia a materiály
3.	Ing. Michal Hičák	Prírodovedecká fakulta UK	4.1.15 anorganická chémia

4.	Ing. Stanislav Mikušínek	Slovenská technická univerzita v Bratislave	5.2.19 anorganická technológia a materiály
5.	Daniel Moreno Rodriguez	Slovenská technická univerzita v Bratislave	5.2.19 anorganická technológia a materiály
6.	Ing. Michal Slaný	Fakulta chemickej a potravinárskej technológie STU	5.2.19 anorganická technológia a materiály

Interní doktorandi hrazení z iných zdrojov*organizácia nemá interných doktorandov hrazených z iných zdrojov***Externí doktorandi***organizácia nemá externých doktorandov***Zoznam zamestnancov prijatých do jedného roka od získania PhD.**

	Meno s titulmi	Dátum obhajoby	Dátum prijatia	Úväzok (v %)
1.	Mgr. Silvia Belušáková, PhD.	22.8.2017	26.8.2017	100

Zoznam emeritných vedeckých zamestnancov**Meno s titulmi**

Príloha B - Projekty riešené v organizácii**Medzinárodné projekty****Programy: Medziakademická dohoda (MAD)****1.) Využitie organo-modifikovaných vrstevnatých silikátov ako nosičov nanočastíc kovov**
(*Immobilization of metal nanoparticles on organo-modified layered silicates*)

Zodpovedný riešiteľ: Helena Pálková
Trvanie projektu: 1.1.2016 / 31.12.2018
Evidenčné číslo projektu: MAD 12/2016
Organizácia je áno
koordinátorom projektu:
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 1 - Poľsko: 1
Čerpané financie: -

Dosiahnuté výsledky:

V rámci spoločného projektu pokračovali experimenty zamerané na modifikáciu ílových minerálov zo skupiny smektitov rôznymi organickými kationmi, ako napríklad tetraalkylfosfóniovými a amóniovými ako aj polymérnym polykationom polydiallyldimethylamóniovým (PDDA). Vzorky sa využili/využijú ako nosiče pre nanočastice kovov. V nadväznosti na experimenty z predchádzajúcich období, v ktorých sa PDDA-modifikovaný smektit použil ako nosič nanočastíc ruténia Ru(0) pre využitie v katalytických reakciách, sa tie isté vzorky použili ako nosiče pre nanočastice striebra Ag(0). Plánované sú testy na antibakteriálnu aktivitu pripravených vzoriek. Pre optimalizáciu celého procesu sa vzorky pripravili rôznymi spôsobmi, Ag(I) sa redukoval v rôznych etapách syntézy, aby sa zistil jeho vplyv na výsledné vlastnosti vzoriek.

Publikácia:

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).

Príspevky na konferenciách:

PÁLKOVÁ, Helena - ZIMOWSKA, Malgorzata - JANKOVIČ, Ľuboš - SERWICKA, Ewa M. - MADEJOVÁ, Jana. Thermo-IR spectroscopy in the study of montmorillonite modified with tetrabutyl-ammonium and phosphonium cations. ICC 2017. International Clay Conference, Granada, Spain. In Scientific Research Abstracts. Digilabs Pub. Italy, 2017, vol. 7, p. 605.

M. ZIMOWSKA, H. PÁLKOVÁ, D. DURACZYŃSKA, L. LITYŃSKA-DOBRYŃSKA, G. MORDARSKI, Ľ. JANKOVIČ, J. MADEJOVÁ, E.M. SERWICKA, Organo-clays as supports for immobilization of ruthenium nanoparticles and their application in 2-butanone hydrogenation. XLIX Ogólnopolskie Kolokwium Katalityczne, Krakow, Poľsko, 15.-17. 3. 2017 (prednáška)

Programy: Medzivládna dohoda**2.) Transparentná oxidová keramika s dodatočnými optickými funkcionalitami** (*Transparent oxide ceramics with additional optical functionalities*)

Zodpovedný riešiteľ: Dušan Galusek
Trvanie projektu: 1.1.2016 / 31.12.2018
Evidenčné číslo projektu: SAS - MOST JRP 2015/06
Organizácia je áno
koordinátorom projektu:
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 1 - Taiwan: 1
Čerpané financie: -

Podpora medzinárodnej spolupráce z národných zdrojov: 24998 €

Dosiahnuté výsledky:

Dosiahnuté výsledky: Skúsenosti získané riešiteľským kolektívom v oblasti dvojstupňového spekania korundovej keramiky so submikrónovou mikroštruktúrou a s prídavkom dopantov ovplyvňujúcich energetické pomery na hraničniciach zŕn sa využili pri príprave plne hutnej transparentnej korundovej keramiky s priemernou veľkosťou zŕn na úrovni 300 – 400 nm použitím kombinácie dvojstupňového spekania a žiarového izostatického lisovania. V rámci spolupráce s CEITEC Brno sa tieto poznatky aplikovali do prípravy korundovej keramiky dopovanej prvkami vzácnych zemín (Eu, Er), s vysokou transparentnosťou vo viditeľnej oblasti (in line transmisia > 50 %) a intenzívnou luminiscenciou v červenej oblasti spektra. Dvojstupňový režim predpekovania vedie k vyššej homogenite distribúcie opticky aktívnych dopantov, zabraňuje tvorbe precipitátov sekundárnej fázy na hraniciach zŕn a zvyšuje transparentnosť pripravených materiálov vo viditeľnej oblasti spektra.

DRDLÍKOVÁ, K. - KLEMENT, Róbert - DRDLÍK, Daniel - SPUSTA, Tomáš - GALUSEK, Dušan - MACA, Karel. Luminescent Er³⁺ doped transparent alumina ceramics. In Journal of the European Ceramic Society, 2017, vol.37, no. 7, p. 2695-2703. (3.454 - IF2016)

DRDLÍKOVÁ, K. - KLEMENT, Róbert - HADRABA, Hynek - DRDLÍK, Daniel - GALUSEK, Dušan - MACA, Karel. Luminescent Eu³⁺-doped transparent alumina ceramics with high hardness. In Journal of the European Ceramic Society, 2017, vol. 37, no. 14, p. 4271-4277. (3.454 - IF2016).

Programy: COST**3.) Naša história z astrochémie (Our Astro-Chemical History)**

Zodpovedný riešiteľ:	Jozef Noga
Trvanie projektu:	26.11.2014 / 25.11.2018
Evidenčné číslo projektu:	CMST COST Action CM1401
Organizácia je koordinátorom projektu:	nie
Koordinátor:	Institut de Planétologie et d'Astrophysique de Grenoble
Počet spoluriešiteľských inštitúcií:	9 - Rakúsko: 1, Česko: 1, Nemecko: 1, Dánsko: 1, Fínsko: 1, Maďarsko: 1, Írsko: 1, Taliansko: 1, Holandsko: 1
Čerpané financie:	-
	Podpora medzinárodnej spolupráce z národných zdrojov: 3150 €

Dosiahnuté výsledky:

Dosiahnuté výsledky: V spolupráci s francúzskym a holandským partnerom sa v roku 2017 kompletizovali výpočty neelastických kolízií atómu uhlíka s molekulou vodíka za pomoci potenciálových hyperplôch napočítaných v predchádzajúcich rokoch. Výsledky, ktoré by sa mali publikovať v r. 2018 sú zaujímavé z hľadiska pochopenia počiatočných štádií kreovania galaxií. V roku 2017 bola tiež publikovaná práca o izomerácii cyklopropánu.

Publikácie:

LANG, Jakub - ŠVAŇA, Matej - DEMEL, Ondřej - BRABEC, Jiří - KEDŽUCH, Stanislav - NOGA, Jozef - KOWALSKI, Karol - PITTNER, Jiří. A MRCC study of the isomerisation of cyclopropane. In Molecular Physics, 2017, vol. 115, no. 21-22, p. 2743-2754. (1.870 - IF2016). (2017 - Current Contents). ISSN 0026-8976. Typ: ADCA

4.) Nová generácia biomimetických implantátov pre náhradu kostí (New generation biomimetic and customized implants for bone engineering)

Zodpovedný riešiteľ:	Pavol Šajgalík
Trvanie projektu:	1.2.2014 / 31.10.2017
Evidenčné číslo projektu:	MPNS COST Action MP1301
Organizácia je koordinátorom projektu:	nie
Koordinátor:	Belgium Ceramic Research Centre Mons
Počet spoluriešiteľských inštitúcií:	56 - Rakúsko: 0, Belgicko: 1, Kanada: 1, Nemecko: 3, Dánsko: 2, Španielsko: 5, Fínsko: 1, Francúzsko: 14, Veľká Británia: 6, Švajčiarsko: 1,

Čerpané financie: Írsko: 2, Island: 1, Taliansko: 6, Litva: 1, Lotyšsko: 1, Holandsko: 2, Nórsko: 0, Portugalsko: 5, Slovinsko: 1, Švédsko: 2, USA: 1
-
Podpora medzinárodnej spolupráce z národných zdrojov: 2625 €

Dosiahnuté výsledky:

V rámci riešenia projektu boli pomocou vymrazovacej granulácie pripravené granuláty na báze nitridu kremičitého. Zmenou zloženia suspenzie (pomer voda:keramický prášok, prídavok granulačných aditív) ako aj zmenou rýchlosti rozstrekovania do kvapalného dusíka bolo možné pripraviť granule s rôznou distribúciou ako veľkosti granúl (20 - 300 μm), tak aj ich pórovitosti. Následnou tlakovou infiltráciou a kalcináciou boli takto pripravené granule povlakované, v celom objeme, hydroxyapatitom. V spolupráci s LF UK boli vykonané testy biokompatibility a bioaktivity. Bioaktivita bola stanovovaná štandardizovaným postupom v simulovanej telesnej tekutine (SBF); z koncentračných zmien hlavných zložiek Ca a P v SBF pred a po teste sa potvrdila tvorba HA na povrchu granúl.

Publikácie:

FENCLOVÁ, Taťána - JONŠTA, Zdeněk - HNATKO, Miroslav - KRAXNER, Jozef. Příprava mikrokuliček z Si₃N₄ pro lékařské použití = Preparation of Si₃N₄ microspheres for medical use. In Interakcie tavenín s progresívnymi anorganickými materiálmi. - Bratislava : Slovenská technická univerzita v Bratislave, 2017, p. 61-69. ISBN 978-80-227-4743-1.(Interakcie tavenín s progresívnymi anorganickými materiálmi).

Programy: Multilaterálne - iné

5.) Relativistické efekty v molekulových materiáloch založených na komplexoch zlata: katalytická aktivita, prenos protónov a NMR vlastnosti (*Relativistic effects in molecular materials based on gold complexes: catalytic activity, proton transfer, and NMR properties*)

Zodpovedný riešiteľ: Oľga Malkin
Trvanie projektu: 1.1.2017 / 31.12.2018
Evidenčné číslo projektu:
Organizácia je áno
koordinátorom projektu:
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 2 - Rakúsko: 1, Česko: 1
Čerpané financie: -
Podpora medzinárodnej spolupráce z národných zdrojov: 1647 €

Dosiahnuté výsledky:

V rámci prvej fázy projektu GOLDCAT sme implementovali poruchovú teóriu tretieho rádu určenú na analýzu spin-orbitálnych príspevkov do NMR chemického posunu. Hlavným výsledkom bolo pochopenie HALA efektu z pohľadu chemickej konfigurácie študovaných systémov. Článok popisujúci túto techniku je v záverečnom štádiu prípravy (J. Vícha, S. Komorovsky, M. Repisky, R. Marek, M. Straka, "Understanding of the SO-HALA Chemical Shifts Across the Periodic Table", v príprave).

Programy: Bilaterálne - iné

6.) Nové technológie pri výrobe hliníka - Fyzikálno-chemické a elektrochemické skúmanie sľubných draselných kryolitových sústav (*New technology in Aluminium production – Physicochemical and electrochemical investigation of promising potassium cryolite molten systems*)

Zodpovedný riešiteľ: Blanka Kubíková
Trvanie projektu: 1.1.2016 / 31.12.2017
Evidenčné číslo projektu: SK-CN-2015-0014
Organizácia je áno
koordinátorom projektu:
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 1 - Čína: 1

Čerpané financie:

-
Podpora medzinárodnej spolupráce z národných zdrojov: 3568 €

Dosiahnuté výsledky:

V druhom roku riešenia projektu bol sledovaný vplyv prídavku LiF a Al₂O₃ na teploty primárnej kryštalizácie v roztavenom systéme KF-AlF₃ pri troch vybraných kryolitových pomeroch. Výsledky ukázali, že pri každom kryolitovom pomere je priebeh závislostí rôzny. Prídavok LiF zvyšuje i znižuje teplotu primárnej kryštalizácie, v jednom prípade bol v študovanom koncentračnom intervale pozorovaný pokles a následný nárast hodnôt teplôt primárnej kryštalizácie. Z porovnania sústav s a bez prídavku Al₂O₃ v tavenine KF-AlF₃ vyplýva, že 5hmot.% Al₂O₃ znižuje teploty primárnej kryštalizácie vo všetkých študovaných zmesiach.

Publikácie a konferenčné príspevky:

KUBÍKOVÁ, Blanka - MLYNÁRIKOVÁ, Jarmila - BOČA, Miroslav – SHI, Zhongning – GAO, Bingliang. Temperatures of primary crystalization and density of KF-AlF₃-LiF-Al₂O₃ molten system. Zaslané do New Journal of Chemistry.

MLYNÁRIKOVÁ, Jarmila - KUBÍKOVÁ, Blanka - BOČA, Miroslav. Vplyv Al₂O₃ a LiF na vlastnosti nízkotopiacich sa elektrolytov na báze KF-AlF₃ systémov. In ChemZi : Slovenský časopis o chémii pre chemické vzdelávanie, výskum a priemysel, 2017, roč. 13, č. 1, s. 163. ISSN 1336-7242.

Programy: ERANET**7.) Kompozity keramika-grafénové platničky pre využitie v tribologických systémoch pracujúcich vo vodnom prostredí** (*Graphene-ceramic composites for tribological application in aqueous environments*)**Zodpovedný riešiteľ:**

Pavol Šajgalík

Trvanie projektu:

1.9.2014 / 31.8.2017

Evidenčné číslo projektu:**Organizácia je**

nie

koordinátorom projektu:**Koordinátor:**

Ústav anorganickej chémie SAV

Počet spoluriešiteľských

0

inštitúcií:**Čerpané financie:**

-
Podpora medzinárodnej spolupráce z národných zdrojov: 6500 €

Dosiahnuté výsledky:

V rámci riešenia projektu boli merané a vyhodnocované funkčné, mechanické a tribologické vlastnosti na pripravených kompozitných materiáloch na báze SiC so spekáciami prísadami oxidom yttritým a oxidom hlinitým a prídavkom 1, 3 a 5 hm. % grafénových nanoplátčiek a 1 hm. % oxidu grafénu. Bola preukázaná výrazná anizotropia elektrickej vodivosti a aj tepelnej difuzivity v závislosti od preferenčného uloženia grafénových vrstiev. Najvýraznejší nárast elektrickej vodivosti sa prejavil vo vzorkách s oxidom grafénu, čo bolo spôsobené procesom prípravy oxidu grafénu a taktiež procesom prípravy samotného kompozitného materiálu, pri ktorom sa podarilo dosiahnuť homogénnu distribúciu grafénových vrstiev v materiály a ich efektívnejšiu delamináciu.

Tepelná difuzivita pripravených materiálov SiC-grafén bola meraná v rozsahu od RT do 400°C, zlepšenie tepelnej difuzivity sa podarilo dosiahnuť v smere rovnobežnom na grafénové vrstvy, pričom tieto pôsobili ako dodatočné fonónové dráhy. Naopak v smere kolmom na grafénové vrstvy došlo k poklesu tepelnej difuzivity v dôsledku rozhraní medzi grafénom a keramickou maticou, ktoré pôsobili ako miesta rozptylu fonónov. Na vzorkách s prídavkom grafénových nanoplátčiek a oxidu grafénu boli merané mechanické vlastnosti (tvrdosť, lomová húževnatosť a Youngov modul pružnosti) v smere kolmom a rovnobežnom na preferenčné uloženie grafénových vrstiev. Tvrdosť materiálov klesala so zvyšujúcim sa prídavkom grafénu ako dôsledok jeho nižšej tvrdosti v porovnaní s maticou. Anizotropia vlastností bola zistená predovšetkým u modulu pružnosti a lomovej húževnatosti. V oboch prípadoch v smere rovnobežnom na grafénové vrstvy boli dosiahnuté vyššie hodnoty meraných vlastností čo možno vysvetliť v prípade lomovej húževnatosti tým, že orientované grafénové platničky bránili šíreniu trhlin a v prípade modulu pružnosti tým že vlastný modul pružnosti grafénu pozdĺž vrstiev je veľmi vysoký (okolo 1 TPa).

Publikácie:

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. (3.411 - IF2016). ISSN 0955-2219 Typ: ADCA

HANZEL, Ondrej - LENČEŠ, Zoltán - KIM, Young-Wook - ŠAJGALÍK, Pavol. Preparation and properties of SiC-Y2O3-Sc2O3 composites with graphene = Příprava a vlastnosti SiC-Y2O3-Sc2O3 kompozitov s prídavkom grafénu. In Workshop Processing and properties of advanced ceramics, November 08-10, 2017, Vrátna-Belá, Slovak Republic : book of extended abstracts. p. 3-9. ISBN 978-80-8075-786-1.

Programy: Horizont 2020

8.) Vývoj nových vysokoteplotných kompozitných materiálov s keramickou maticou so zvýšenou oxidačnou/ablačnou odolnosťou pre vesmírne aplikácie (*Development of new ultra-high temperature ceramic matrix composites with improved oxidatio/ablation properties for aerospace industry*)

Zodpovedný riešiteľ: Peter Tatarko
Trvanie projektu: 1.11.2017 / 31.10.2020
Evidenčné číslo projektu: MVTs 41090027
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: -
 Podpora medzinárodnej spolupráce z národných zdrojov: 4000 €

Dosiahnuté výsledky:

Projekt sa na ÚACH rieši len od novembra 2017, z toho dôvodu momentálne nie je možné informovať o výsledkoch. Úvodná fáza projektu bola venovaná plánovaniu a príprave experimentálnych postupov riešenia projektu.

Projekty národných agentúr

Programy: VEGA

1.) Roztavené fluoridové systémy s vyššou funkcionalitou (*Molten fluoride systems with higher functionality*)

Zodpovedný riešiteľ: Miroslav Boča
Trvanie projektu: 1.1.2016 / 31.12.2019
Evidenčné číslo projektu: 2/0114/16
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 20780 €

Dosiahnuté výsledky:

Predmetom systematického výskumu taveninových sústav NaF/LiF/KF/-K2TaF7 bola hustota a ich objemové vlastnosti, ktoré patria k základným fyzikálno-chemickým vlastnostiam tavenín. Dosiahnuté výsledky boli porovnávané s analogickými systémami NaF/LiF/KF/-K2NbF7 a ukázali, že molárny objem monotónne rastie so zvyšujúcim sa obsahom K2TaF7 resp. K2NbF7 vo všetkých skúmaných sústavách. Negatívne hodnoty dodatkového objemu poukazujú na objemovú kontrakciu v sústavách s K2TaF7 i K2NbF7. Rozdielne správanie študovaných sústav však bolo pozorované v prípade parciálneho dodatkového objemu, kde v prípade sústav s K2TaF7 bola potvrdená objemová kontrakcia kationov alkalických kovov, narozdiel od sústav s K2NbF7, kde bola pozorovaná ich objemová expanzia. Výsledky skúmania objemových vlastností týmto odzrkadľujú interakcie iónov v roztavenom stave.

MLYNÁRIKOVÁ, Jarmila - BOČA, Miroslav - MIKŠÍKOVÁ, Eva - NETRIOVÁ, Zuzana. Volume properties of the molten systems MF-K2TaF7 (MF = LiF, NaF and KF). In Journal of Thermal Analysis and Calorimetry, 2017, vol. 129, no. 1, p. 475-486. (1.953 - IF2016). ISSN 1388-6150.)

Ďalšou oblasťou výskumu bolo sledovanie vplyvu agresívnych roztavených solí na vybrané kovové zliatiny. Súhrnný prehľadný článok sumarizuje výsledky množstva autorov pre rôzne typy agresívnych prostredí. Výsledky z korózneho

správania niklových superzliatin v sústave LiF-NaF-KF sú v oponentskom procese.

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. (6.455 - IF2016). ISSN 1040-8436.

2.) Fotoaktívne hybridné materiály (*Photoactive hybrid materials*)

Zodpovedný riešiteľ: Adriana Czímerová
Trvanie projektu: 1.1.2017 / 31.12.2020
Evidenčné číslo projektu: 2/0156/17
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 6033 €

Dosiahnuté výsledky:

Projekt sa začal riešiť v roku 2017. V tejto počiatočnej fáze boli vybrané vhodné ílové minerály a farbivá na prípravu hybridných materiálov. Študoval sa hlavne vplyv rozpúšťadiel, množstva ílového minerálu a koncentrácia farbív na vznik hybridných materiálov s luminescenčnými vlastnosťami. Navyše sa pripravili tenké vrstvy ílových minerálov, polymérov a farbív metódami tzv. „layer-by-layer assembly“ a pomocou Langmuir-Blodgettovej techniky. Pripravené filmy vykazovali luminescenčné vlastnosti, navyše v oboch prípadoch bol dokázaný jav prenosu energie. Pripravené filmy boli kompletne charakterizované pomocou absorpčnej spektroskopie vo viditeľnej oblasti spektra a fluorescenčnou spektroskopiou.

Dosiahnuté výsledky:

CZÍMEROVÁ, Adriana - SAS, Samuel - ČEKLOVSKÝ, Alexander. Unique solvatochromism of cyanine/saponite hybrid systems. In Applied Clay Science, 2017, vol. 141, p. 198-203. (3.101 - IF2016).

CZÍMEROVÁ, Adriana - ČEKLOVSKÝ, Alexander. Resonance energy transfer between rhodamine dyes in saponite thin films: a step towards novel photofunctional nanohybrids. In Clay Minerals, 2017, vol. 52, p. 263-273. (1.052 - IF2016).

3.) Transparentné polykryštalické keramické materiály so submikrónovou mikroštruktúrou a luminescenčnými vlastnosťami (*Transparent polycrystalline ceramics materials with submicrone microstructure and with luminiscent properties*)

Zodpovedný riešiteľ: Dušan Galusek
Trvanie projektu: 1.1.2017 / 31.12.2020
Evidenčné číslo projektu: 2/0026/17
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 7298 €

Dosiahnuté výsledky:

V rámci projektu sa aktivity zameriavali na prípravu transparentných materiálov na báze ytrito-hlinitého granátu (YAG) žiarovým lisovaním sklenených mikroguličiek identického zloženia. V rámci toho sa detailne skúmala kinetika kryštalizácie skiel v systéme Al₂O₃-Y₃Al₅O₁₂. Na základe popisu procesu kryštalizácie pomocou JMAK modelu (Johnson-Mehl-Avrami –Kolmogorov) sa stanovili mechanizmy a kinetika kryštalizácie u systémov s eutektickým zložením, zložením blízkym binárnemu eutektiku Al₂O₃-Y₃Al₅O₁₂ a čistej YAG fázy. Získané poznatky sa využili pre prípravu translucetnej polykryštalickej YAG keramiky a polykryštalických keramických materiálov v systéme Al₂O₃-YAG so submikrónovou mikroštruktúrou so vzájomne perkolujúcimi fázami (tzv. eutektická mikroštruktúra). Vedľajším produktom bola príprava dutých polykryštalických YAG mikriguličiek použiteľných ako médium pre rádioterapiu nádorových ochorení.

PRNOVÁ, Anna - KLEMENT, Róbert - BODIŠOVÁ, Katarína - VALÚCHOVÁ, Jana - GALUSEK, Dušan - BRUNEEL, E. - VAN DRIESSE, I. 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, 2017, vol. 128, no. 3, p. 1407-1415. (1.953 - IF2016)

CHOVANEK, J. - SVOBODA, R. - KRAXNER, J. - ČERNÁ, A. - GALUSEK, D. Crystallization kinetics of the Y3Al5O12 glass, Journal of Alloys and Compounds 725 (2017) 792-799, doi: 10.1016/j.jallcom.2017.07.191

KRAXNER, Jozef - CHOVANEK, Jozef - HALADEJOVÁ, Katarína - PETRÍKOVÁ, I. - GALUSEK, Dušan. Hollow polycrystalline YAG microspheres by flame synthesis. In Materials Letters, 2017, vol. 204, p. 181-183. (2.572 - IF2016).

PRNOVÁ, Anna - PLŠKO, A. - VALÚCHOVÁ, Jana - HALADEJOVÁ, K. - KLEMENT, Róbert - GALUSEK, Dušan, I. Crystallization kinetics of glass microspheres with yttrium aluminium garnet (YAG) composition, Journal of Thermal Analysis and Calorimetry vol. 113 num. 3 (2017) 6690-6900, doi: 10.1007/s10973-017-6690-9

4.) Zlepšenie funkčných vlastností keramických materiálov prídavkom uhlíkových nanorúrok a grafénu (*Improvement of functional properties of ceramic materials with the addition of carbon nano-tubes and graphene*)

Zodpovedný riešiteľ:	Miroslav Hnatko
Trvanie projektu:	1.1.2014 / 31.12.2017
Evidenčné číslo projektu:	2/0065/14
Organizácia je koordinátorom projektu:	áno
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	0
Čerpané financie:	SAV: 7591 €

Dosiahnuté výsledky:

Za posledné obdobie sa v rámci riešenia projektu podarilo pripraviť hutný (99% teoretickej hustoty) karbid kremičitý s prídavkom GNPs (GrapheneNanoPlatelets) a GO (GrapheneOxide) metódou RHP (rapidhot press). Prídavok GNPs a špeciálne prídavok GO viedol k výraznému zvýšeniu elektrickej vodivosti (viac ako 17 krát vyšie hodnoty v porovnaní s referenčným SiC). Zlepšenie elektrickej vodivosti bolo dosiahnuté vďaka zvládnuť technológii prípravy, predovšetkým optimalizáciou procesu delaminácie GO a dokonalou homogenizáciou častíc grafénu v objeme SiC matrice.

Publikácie:

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. (3.411 - IF2016). ISSN 0955-2219. ADCA

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. (3.411 - IF2016). ISSN 0955-2219. ADCA

HNATKO, Miroslav - SEDLÁČEK, Jaroslav - LÁZÁR, Marián. Zhodnocovanie vitrifikovanej trosky z plazmo-termického spracovania odpadov - príprava pórovitej sklo-keramickej matrice = Upgrading of vitrified slag from waste disposal by thermal plasma treatment - formation of porous glass-ceramic matrix. In Interakcie tavenín s progresívnymi anorganickými materiálmi. - Bratislava : Slovenská technická univerzita v Bratislave, 2017, p. 103-112. ISBN 978-80-227-4743-1.(Interakcie tavenín s progresívnymi anorganickými materiálmi). AEDA

5.) Štruktúra a vlastnosti oxidových skiel - termodynamický model, entalpická a objemová relaxácia (*Structure and properties of oxide glasses - thermodynamic models, enthalpic and structural relaxation*)

Zodpovedný riešiteľ:	Mária Chromčíková
Trvanie projektu:	1.1.2016 / 31.12.2020
Evidenčné číslo projektu:	2/0088/16

Organizácia je koordinátorom projektu:	áno
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	1 - Slovensko: 1
Čerpané financie:	SAV: 1786 €

Dosiahnuté výsledky:

Výsledky získané v oblasti parametrizácie a validácie termodynamických modelov boli v spolupráci s VŠChT Praha sumárne kriticky vyhodnotené a opublikované v podobe samostatnej kapitoly v monografii vydanej vydavateľstvom Springer.

6.) Nové anorganické fosfory na báze hlinitanov vzácnych zemín pre aplikácie v LED diódach vyžarujúcich biele svetlo (*New rare-earth aluminate-based inorganic phosphors for applications in white light emitting LEDs*)

Zodpovedný riešiteľ:	Róbert Klement
Trvanie projektu:	1.1.2014 / 31.12.2017
Evidenčné číslo projektu:	1/0631/14
Organizácia je koordinátorom projektu:	nie
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	0
Čerpané financie:	SAV: 4051 €

Dosiahnuté výsledky:

Pripravené boli sklo-polykryštalické fosfory v sústavách $Y_2O_3-Al_2O_3$ a $Y_2O_3-Al_2O_3-SiO_2$ dopované iónmi Ce^{3+} - Mn^{2+}/Mn^{4+} a Eu^{2+}/Eu^{3+} vyžarujúce biele svetlo, so zvýšenou emisiou v červenej spektrálnej oblasti, po excitácii NUV žiarením. Ióny Ce^{3+} zabudované v YAG matici vykazujú žltó-zelenú emisiu, zatiaľ čo ióny vo zvyškovej sklenej fáze modrú emisiu pri excitácii NUV žiarením. Tým možno riadenou kryštalizáciou pripraviť systém emitujúci biele svetlo. Veľmi sľubné výsledky poskytuje systém $Y_2O_3-Al_2O_3$ dopovaný Eu^{2+}/Eu^{3+} iónmi. Vzhľadom na prítomnosť oboch oxidačných stavov Eu v matici (Eu^{2+} intenzívne emituje v oblasti 400-700 nm, Eu^{3+} typický emitér červeného svetla) možno dosiahnuť emisiu bieleho svetla, pričom ladením vlnovej dĺžky excitujúceho žiarenia efektívne zvýšiť podiel emisie červeného svetla vo výslednom bielom svetle. Nespornou výhodou je najmä využitie len jedného RE iónu v pomerne nízkej koncentrácii v matici na rozdiel od známych fosforov kde je na emisiu bieleho svetla nevyhnutná prítomnosť 2-3 rôznych RE iónov v jednej alebo viacerých fázach.

7.) Svetlo emitujúce luminofóry na báze ternárnych nitridov a oxynitridov kremíka (*Ternary silicon nitride and oxynitride-based phosphors*)

Zodpovedný riešiteľ:	Zoltán Lenčes
Trvanie projektu:	1.1.2014 / 31.12.2017
Evidenčné číslo projektu:	2/0112/14
Organizácia je koordinátorom projektu:	áno
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	0
Čerpané financie:	SAV: 12803 €

Dosiahnuté výsledky:

Luminofory na báze $LaSi_3N_5$ a dopované lantanoidmi ($Ln = Ce, Er, Yb$) boli pripravené zo zmesí $LaSi_3N_5/LnF_3$ a $LaSi_3N_5/Ln_2O_3$ žiahaním pri 1600 °C po dobu 3 h v pretlaku dusíka 2 MPa. Luminofory dopované fluoridmi vykazujú pomerne ostré/úzke emisné píky s maximom 546 nm pre CeF_3 -dopovaný materiál, pri 397 nm a 468 nm pre ErF_3 a pri 483 nm pre YbF_3 dopovaný $LaSi_3N_5$ luminofor. V prípade luminoforov $LaSi_3N_5$ dopovaných oxidmi lantanoidov boli namerané výrazne širšie emisné píky (pri 510 – 625 nm pre CeO_2 dopovaný materiál, 370 – 600 nm pre Er_2O_3 , a 440 – 600 nm pre Yb_2O_3 dopovaný materiál). Poloha maxim bola približne rovnaká, ako u luminoforch dopovaných fluoridmi lantanoidov.

Pri príprave luminoforov na báze O'-sialonu ($\text{Si}_{2-x}\text{Al}_x\text{O}_{1+x}\text{N}_{2-x}$, tzn. tuhý roztok $\text{Si}_2\text{N}_2\text{O}$ a Al_2O_3) boli študované dva spôsoby: i) príprava O'-sialonu reakciami v tuhej fáze zo zmesi $\text{Si}_3\text{N}_4 + \text{SiO}_2 + \text{Al}_2\text{O}_3$ a ii) zo zmesi Si_3N_4 a SiAlOC polymérneho prekursoru. Výsledky ukázali, že príprava O'-sialonu reakciami v tuhej fáze je veľmi pomalá a po syntéze prášku pri 1800°C po dobu 2 hodín v pretlaku dusíka (1,5 MPa) produkt pozostával z majoritného Si_3N_4 , $\text{Si}_2\text{N}_2\text{O}$ (20%), minoritného Al_2O_3 a amorfného SiO_2 . Druhú spôsob syntézy je efektívnejší, zo zmesi Si_3N_4 a SiAlOC sa podarilo pripraviť O'-sialon pri nižších teplotách (1750°C) a kratších časoch (15 min). Na zabudovanie dopantu (Eu) do štruktúry O'-sialonu bolo nutné vzorky ďalej žihať pri 1650°C po dobu 2 hodín. Luminofor O'-sialon:Eu emitoval žiarenie v žltej oblasti viditeľného svetla. Intenzita emitovaného žiarenia bola zvýšená dôkladným odstránením (výpalom) uhlíka z SiAlOC polymérneho prekursoru (800°C , 1 h na vzduchu) pred samotným žihaním, lebo zostatkový uhlík v luminofore znižoval intenzitu emitovaného žiarenia.

8.) Funkcionalizácia ílových minerálov netradičnými organickými surfaktantmi (*Functionalization of clay minerals using unconventional organic surfactants*)

Zodpovedný riešiteľ: Jana Madejová
Trvanie projektu: 1.1.2017 / 31.12.2020
Evidenčné číslo projektu: 2/0141/17
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 22791 €

Dosiahnuté výsledky:

V prvom roku riešenia projektu sa zo slovenského bentonitu z lokality Jelšový potok (JP, Slovensko) a z bentonitu získaného z Clay Mineral Society (SAZ, Arizona, USA) vyseparovali jemne frakcie a pripravili Na-formy. Následne sa z nich pripravili rôzne typy alkyl-amóniových a alkyl-fosfóniových organo-derivátov. Z alkylamóniových kationov to boli predovšetkým kationy zo série n-alkylamóniových ($\text{C}_n\text{-NH}_3$, $n=1-19$) kationov, kationy tzv. oktylového radu: monoalkyl- (1C8), dialkyl- (2C8), trialkyl- (3C8) a tetraalkyl- (4C8). Na porovnanie vplyvu centrálného atómu koncovkej skupiny (N vs P) sa pripravili tetrametyl-, tetrabutyl- a tetraalkyl-amóniové a tetrametyl-, tetrabutyl- a tetraalkyl-fosfóniové formy. Na charakterizáciu vzoriek sa využili rôzne metódy, napr. röntgenová difrakcia, IČ spektroskopia v MIR a NIR oblasti, termická (TG/DTA) a chemická analýza. Zistilo sa, že termická stabilita fosfóniových foriem je vyššia ako amóniových foriem. Mechanická stabilita pripravených foriem sa študovala na pripravených formách ich mletím vo vysokoenergetickom planetárnom mlyne. Na základe IČ spektier sa pozorovalo spomalenie rozkladu štruktúry ílového minerálu v prípade organo-modifikovaných vzoriek. Metódou IČ spektroskopie v NIR oblasti sa sledoval vplyv organického kationu a relatívnej vlhkosti na usporiadanie surfaktantov v medzivrstvových priestoroch JP montmorillonitu. Prítomnosť molekúl vody vo vzorkách spôsobuje nárast množstva usporiadaných "trans" a pokles neusporiadaných "gauche" konformérov. Pomocou DFT metódy sa uskutočnili výpočty zamerané na porovnanie stability montmorillonitov a beidelitov interkalovaných tetrabutylamóniovým a tetrabutylfosfóniovým kationom. Začali sa úvodné testy adsorpcie rôznych fluorescenčných farbív, ľahko podliehajúcich molekulovej agregácii, napríklad rodamínov a oxazínov, na sérii organo-modifikovaných ílov.

Publikácie:

BIZOVSKÁ, Valéria - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana. Montmorillonite Modified with Less-traditional Surfactants from the Series of Octylammonium-based Cations: Structural Characterization and Hydration Properties. Applied Clay Science, (CLAY11131, v recenznom konaní).
 SCHOLTZOVÁ, Eva – TUNEGA, D. DFT study of stability of the tetrabutylphosphonium and tetrabutylammonium montmorillonites. Clay Minerals (CM-17-78, v recenznom konaní)

9.) Vývoj pokročilých nástrojov na výpočet a interpretáciu NMR a EPR spektier systémov ťažkých prvkov (*Development of advanced tools for calculation and interpretation of NMR and EPR spectra of heavy element compounds*)

Zodpovedný riešiteľ: Oľga Malkin
Trvanie projektu: 1.1.2017 / 31.12.2020
Evidenčné číslo projektu: 2/0116/17
Organizácia je áno

koordinátorom projektu:**Koordinátor:** Ústav anorganickej chémie SAV**Počet spoluriešiteľských** 0**inštitúcií:****Čerpané financie:** SAV: 13407 €**Dosiahnuté výsledky:**

HAASE, Pi A. B. - REPISKÝ, Michal - KOMOROVSKÝ, Stanislav - BENDIX, Jesper - SAUER, Stephan P. A. Relativistic DFT calculations of hyperfine coupling constants in 5d hexafluorido complexes: [ReF₆]²⁻ and [IrF₆]²⁻. In Chemistry - A European Journal, 2017, vol. 23, p.1521-1-1521-11. (5.317 - IF2016).

NOVOTNÝ, Jan - VÍCHA, Jan - BORA, Pankaj L. - REPISKÝ, Michal - STRAKA, Michal - KOMOROVSKÝ, Stanislav - MAREK, Radek. Linking the character of the metal-ligand bond to the ligand NMR shielding in transition-metal complexes: NMR contributions from spin-orbit coupling. In Journal of Chemical Theory and Computation, 2017, vol. 13, no. 8, p. 3586-3601.

10.) Elektrolyty s nízkou teplotou topenia a zmáčané katódy s potenciálom pre zlepšenie procesu výroby hliníka (*Low melting electrolytes and wetted cathodes with potential for electrolytic aluminium production*)

Zodpovedný riešiteľ: František Šimko**Trvanie projektu:** 1.1.2014 / 31.12.2017**Evidenčné číslo projektu:** 2/0116/14**Organizácia je** áno**koordinátorom projektu:****Koordinátor:** Ústav anorganickej chémie SAV**Počet spoluriešiteľských** 0**inštitúcií:****Čerpané financie:** SAV: 11060 €**Dosiahnuté výsledky:**

Uskutočnila sa štruktúrna a fázová analýza systému RbF-Al₂O₃. Bola stanovená štruktúra druhého známeho oxofluorohlinitanu alkalického kovu, Rb₂Al₂O₃F₂. Pri analýze danej zlúčeniny, ⁸⁵Rb-¹⁹F a ²⁷Al-¹⁹F 2D D-HMQC NMR experimenty potvrdili existenciu dvoch rozdielnych štruktúrnych typov atómov rubidia, jedného štruktúrneho typu atómu hliníka vo forme (AlO₃F) tetraédrov a jedného štruktúrneho typu atómu fluóru. Pri analýzach sa zistila štruktúrna podobnosť kovalentne viazaných FO₂Al-O-AlO₂F tetraédrov v štruktúre Rb₂Al₂O₃F₂ s podobným usporiadaním O₃Al-O-AlO₃ tetraédrov v štruktúre oxohlinitanu mullitového typu, Rb₂O×11Al₂O₃. Tepelná stabilita Rb₂Al₂O₃F₂ a časť fázového diagramu binárneho systému RbF-Al₂O₃ s obsahom Al₂O₃ do 20 mol. % sa skúmala pomocou termickej analýzy. Systém nie je definovaný ako pravý jednoduchý binárny systém, ale ide o stabilnú diagonálu kvartérneho systému RbF-AlF₃-Al₂O₃-Rb₂O. Obsahuje fázy Rb₂Al₂O₃F₂, α-Rb₃AlF₆, RbAlO₂ a Rb₂O×11Al₂O₃, ktoré boli identifikované v analyzovanej časti systému pomocou Rtg práškovej difrakčnej analýzy a NMR spektroskopie. Z fázovej analýzy jednotlivých fázových polí možno vziať do úvahy vzájomné matastabilné správanie sa všetkých uvedených fáz.

Analyzovali sa korózne experimenty zamerané na objasnenie interakcie TiB₂ s roztaveným elektrolytom zloženia 1,3KF-AlF₃ s prídavkom 4,5 hmot.% Al₂O₃, ktorej zloženie je zaujímavé z hľadiska nízkoteplotnej výroby hliníka. Uskutočnili sa statické korózne testy TiB₂ v tavenine pri teplote 680°C po dobu 200 hodín. Korózne produkty boli analyzované pomocou XRD, IR, SEM-EDX a EBSD analytických metód. Tie potvrdili napadnutie zrn TiB₂, ktoré boli v kontakte s koróznym médiom a vznik TiO₂ ako jedného z korózných produktov. Analýza použitej taveniny potvrdila okrem fáz, vznikajúcich reakciou zložiek elektrolytu (K₃AlF₆ a KAlF₄) aj prítomnosť ostatných korózných produktov s obsahom bóru v podobe hlinitoboritanu so (BO₃)³⁻ a (BO₄)⁴⁻ štruktúrnym fragmentami.

Publikácie

ŠIMKO, František - 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. (4.857 - IF2016). ISSN 0020-1669.

ŠIMKO, František - RAKHMATULLIN, Aydar - FLORIAN, Pierre - KONTRÍK, Martin - NETRIOVÁ, Zuzana - BESSADA, Catherine. Fluoro-, oxo-, oxofluoro-aluminates in the system RbF-AlF₃-Al₂O₃-Rb₂O: their stability and structure correlation. In Preparation of ceramic materials : Proceedings of the 12th international conference. Jahodná, 13.-15.6.2017. Ed. B. Plešingerová et al. - Košice : Technical University, 2017, p. 162-163. ISBN

978-80-553-3160-7.(Preparation of ceramic materials : international conference).

ŠIMKO, František - RAKHMATULLIN, Aydar - FLORIAN, Pierre - KONTRÍK, Martin - NETRIOVÁ, Zuzana - BESSADA, Catherine. Oxofluoroaluminates in the system $\text{RbF-AlF}_3\text{-Al}_2\text{O}_3\text{-Rb}_2\text{O}$: thermal stability and structural correlation. In ChemZi : Slovenský časopis o chémii pre chemické vzdelávanie, výskum a priemysel, 2017, roč. 13, č. 1, s. 164-165. ISSN 1336-7242

ŠIMKO, František - RAKHMATULLIN, Aydar - FLORIAN, Pierre - KONTRÍK, Martin - NETRIOVÁ, Zuzana - BESSADA, Catherine. Fluóro-, oxo- a oxofluórohlinitany: stabilita a ich vzájomná štruktúrna korelácia = Fluoro-, oxo-, and oxofluoro-aluminates: stability and structure correlation among them. In Interakcie tavenín s progresívnymi anorganickými materiálmi. Bratislava: Slovenská technická univerzita v Bratislave, 2017, p. 98-99. ISBN 978-80-227-4743-1.(Interakcie tavenín s progresívnymi anorganickými materiálmi).

Programy: APVV

11.) Fluoridové taveniny kritických prvkov pre nekonvenčné aplikácie (*Fluoride melts of critical elements for unconventional applications*)

Zodpovedný riešiteľ: Miroslav Boča
Trvanie projektu: 1.7.2016 / 30.6.2020
Evidenčné číslo projektu: APVV-15-0479
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: APVV: 70000 €

Dosiahnuté výsledky:

Na sústave 41 fluoridových vzoriek obsahujúcich K_2TaF_7 , Na_3AlF_6 , K_2ZrF_6 , NaF, a LiF boli zaznamenávané rtg. fluorescenčné signály. Výsledky ukázali, že výsledná intenzita takéhoto signálu je výsledkom viacerých efektov. Je možné analyzovať "ťažké" i ľahké prvky, avšak je obtiažne určiť podiel jednotlivých efektov a ako sa navzájom ovplyvňujú, prípadne rušia.

Publikácie:

BOČA, Miroslav - GURIŠOVÁ, Veronika - ŠIMKO, František. Some aspects of the wavelength dispersive x-ray determination of fluorine content in various matrices. In Journal of Applied Spectroscopy, 2017, vol. 84, no. 2, 8 p. (0.572 - IF2016). ISSN 0021-9037.

12.) Prevencia a eradikácia mikrobiálnych biofilmov vo vzťahu k nanomateriálom (*Prevention and eradication of microbial biofilms in relationship to nanomaterials*)

Zodpovedný riešiteľ: Juraj Bujdák
Trvanie projektu: 1.7.2016 / 30.6.2020
Evidenčné číslo projektu: APVV-15-0347
Organizácia je koordinátorom projektu: nie
Koordinátor: Prírodovedecká fakulta UK
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: APVV: 22000 €

Dosiahnuté výsledky:

Hlavnou úlohou kolektívu UACH v projekte bola príprava a charakterizácia hybridných nanomateriálov s antimikrobiálnymi vlastnosťami. Hlavným typom boli materiály s fotosenzibilizačnými vlastnosťami (1). Pre tento typ materiálov bolo dôležité pochopiť základné zákonitosti pre efektívne využitie svetelnej energie na fotoaktiváciu kyslíka a elimináciu niektorých nežiaducich konkurenčných javov. V tomto kontexte vznikli práce, ktoré sa zaoberajú najmä fotofyzikálnymi vlastnosťami takýchto hybridných sústav (2-4). Začali sme sa tiež zaoberať aj vývojom ďalších typov materiálov s biocídnymi vlastnosťami, zahŕňajúce napr. antibiotiká, nanočastice kovov a niektoré polymérne látky.

1. RIAZ, Ufana - ASHRAF, S. M. - BUJDÁK, Juraj. Recent advances in nano photodynamic therapy : Chapter 6. In Recent advances in analytical techniques. - UAE, Sharjah : Bentham Science Publishers, 2017, vol. 1, p. 200-223. ISBN 978-1-68108-448-0.
2. 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.
3. BUJDÁK, Juraj. Hybrids with functional dyes : Chapter 18. In Inorganic nanosheets and nanosheet-based materials : Fundamentals and applications of two-dimensional systems. - Tokyo, Japan : Springer Japan, 2017, p. 419-465. ISBN 978-4-431-56494-2. ISSN 1571-5744.
4. SAS, Samuel - DANKO, Martin - BIZOVSKÁ, Valéria - LANG, Kamil - BUJDÁK, Juraj. Highly luminescent hybrid materials based on smectites with polyethylene glycol modified with rhodamine fluorophore. In Applied Clay Science, 2017, vol. 138, p. 25-33. (3.101 - IF2016). ISSN 0169-1317.

13.) Keramické materiály pre použitie v extrémnych podmienkach (*Ceramic materials for extreme operating conditions*)

Zodpovedný riešiteľ:	Ján Dusza
Zodpovedný riešiteľ v organizácii SAV:	Pavol Šajgalík
Trvanie projektu:	1.7.2016 / 30.6.2020
Evidenčné číslo projektu:	APV-15-0469
Organizácia je koordinátorom projektu:	nie
Koordinátor:	Ústav materiálového výskumu SAV
Počet spoluriešiteľských inštitúcií:	0
Čerpané financie:	APVV: 22000 €

Dosiahnuté výsledky:

ÚACH, ako spoluriešiteľská organizácia, je zodpovedná za vývoj nových diboridových keramických materiálov pre aplikácie pracujúce v extrémnych podmienkach. V tomto roku boli hlavné aktivity venované vývoju kompozitných materiálov na báze TiB₂-SiC. To zahŕňa, štúdium rôznych spôsobov prípravy práškových zmesí a následného spekania práškov pomocou modernej technológie, tzv. spekania za asistencie elektrického prúdu (electric current assisted sintering technology). Pri riešení bol nájdený optimálny spôsob prípravy práškovej zmesi, pozostávajúci z homogenizácie vstupných práškov v isopropanole pomocou planetového mlynu (mlecie médium a podmienky mletia boli optimalizované) a následného odparovania isopropanolu pomocou vákuovej rotačnej odparky. Zhutňovanie a process spekania boli podrobne analyzované pri rôznych podmienkach, pričom ako optimálne podmienky spekania boli určené nasledovné: teplota 2100°C, tlak 90 MPa, doba výdrže na max. teplote 7 min, rýchlosť ohrevu a chladenia 100°C/min, atmosféra Ar. Nakoľko si projekt dáva za cieľ zlepšiť vlastnosti diboridovej keramiky pomocou prídavku grafénových nanoplátčiek, ich prídavok na process spekania a vývin mikroštruktúry kompozitov TiB₂-SiC bol taktiež študovaný v tomto roku. Celkovo bola pripravená celá séria referenčných materiálov TiB₂-SiC s rôznym obsahom SiC a taktiež celá séria TiB₂-SiC materiálov s rôznym obsahom grafénových nanoplátčiek (1, 2, 5, a 10 hm.%). V rámci štúdie bol taktiež skúmaný vplyv 2 odlišných druhov grafénových nanoplátčiek. Vplyv týchto prísad bol hodnotený s ohľadom na spekanie materiálov, teoretickej hustoty, vývoj mikroštruktúry a fáz v mikroštruktúre.

Publikácie:

TATARKO, Peter - GRASSO, Salvatore - SAUNDERS, Theo G. - FERRARIS, Monica - REECE, Michael J. Flash joining of CVD-SiC coated Cf/SiC composites with a Ti interlayer. In Journal of the European Ceramic Society, 2017, vol. 37, no. 13, p. 3841-3848. (3.411 - IF2016). ISSN 0955-2219. ADCA

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. (3.411 - IF2016). ISSN 0955-2219. ADCA

SEDLÁK, Richard - KOVALČÍKOVÁ, Alexandra - MÚDRA, Erika - RUTKOWSKI, Pawel - DUBIEL, Aleksandra - GIRMAN, Vladimír - BYSTRICKÝ, Roman - DUSZA, Ján. Boron carbide/graphene platelet ceramics with improved fracture toughness and electrical conductivity. In Journal of the European Ceramic Society, 2017, vol. 37, p. 3773-3780. (3.411 - IF2016). ISSN 0955-2219. ADCA

14.) Kompozitné vrstvy pre vysokoteplotnú protikoróznú ochranu kovov (*Advanced composite coatings*)

for high temperature corrosion protection of metals)

Zodpovedný riešiteľ: Dušan Galusek
Trvanie projektu: 1.7.2016 / 30.6.2020
Evidenčné číslo projektu: APVV-15-0014
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 2 - Slovensko: 2
Čerpané financie: APVV: 22500 €

Dosiahnuté výsledky:

V rámci projektu sa pripravili hrubé (max. hrúbka do 100 µm) vrstvy s keramickou maticou (kombinácia amorfnej keramiky pripravenej termickým rozkladom organokremičitých polymérov – polysilazánov a YSZ) so sklenými plnivami. Sklené plnivá sa pridávali vo forme sklených mikroguličiek v ťažko taviteľných systémoch s vysokou teplotou mäknutia, napr. Al₂O₃-Y₂O₃, alebo Al₂O₃-SiO₂-ZrO₂, ktorých úlohou je čiastočne eliminovať zmraštenie keramickej matrice pri jej vzniku z polymérneho prekursora, alebo komerčných sklených frít s nižšou teplotou tavenia, ktoré pri teplote použitia mäknú a zabezpečujú vyhojovanie prípadných defektov v keramickej matrici. Vrstvy sa aplikovali na povrch nerezovej ocele AISI 411 a testovali z hľadiska adhézie na kovovom substrate a ich odolnosti voči korózii v prostredí subkritickej vody a horúcej oxidačnej atmosféry s vysokým obsahom vodnej pary. Pripravené vrstvy zvyšujú odolnosť nerezovej ocele voči oxidácii pri teplotách do 900 °C. Pri vyšších teplotách ako aj pri vysokých parciálnych tlakoch vodnej pary je ochranný efekt zanedbateľný.

PARCHOVIANSKÝ, Milan - BALKO, Ján - ŠVANČÁREK, P. - SEDLÁČEK, Jaroslav - DUSZA, Ján - LOFAJ, František - GALUSEK, D. Mechanical properties and sliding wear behaviour of Al₂O₃-SiC nanocomposites with 3-20 vol% SiC. In Journal of the European Ceramic Society, 2017, vol. 37, p. 4297-4306. (3.454 - IF2016).

LEITE M.L. – BARROSO, G. – PARCHOVIANSKÝ – GALUSEK, D. – IONESCU E. – KRENKEL W. – MOTZ G. Synthesis and characterization of yttrium and ytterbium silicates from their oxides and an oligosilazane by the PDC route for coating applications to protect Si₃N₄ in hot gas environments, Journal of the European Ceramic Society 37 (2017) 5177–5191, doi: 10.1016/j.jeurceramsoc.2017.04.034.

15.) Zhodnotenie druhotných surovín pre materiály s využitím v extrémnych podmienkach
(Assessment of secondary raw materials for the preparation of materials used in extreme conditions)

Zodpovedný riešiteľ: Miroslav Hnatko
Trvanie projektu: 1.7.2016 / 30.6.2020
Evidenčné číslo projektu: APVV-15-0540
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: APVV: 43777 €

Dosiahnuté výsledky:

V procese výberu odpadov ako potenciálnych druhotných surovín bolo vybratých 21 rôznych zdrojov pochádzajúcich zo súčasnej produkcie firiem (OFZ a.s., US Steel Košice s.r.o.), spaľovania komunálneho odpadu (OLO a.s.) ako aj existujúcich skládok predstavujúcich environmentálnu záťaž (OFZ a.s., Niklové hute Sereď). Selekcia prebiehala na základe chemického a fázového zloženia, tak aby bolo možné ich kombináciou meniť nielen finálne zloženie, ale najmä ich spracovateľnosť z pohľadu projektového zámeru. Z pohľadu chemického zloženia sú jednotlivé zdroje odpadov majoritne na báze oxidov kremíka, hliníka, vápnika, horčíka a železa (zastúpených v rôznych pomeroch). Vyselektované odpady boli podrobené detailnej termickej analýze, ktorá v kombinácii s fázovým zložením poskytuje informácie o teplotnom interval spracovania samotnej druhotnej suroviny, resp. v prípade ich kombinácie a prípadne prídavku ďalších zložiek predikuje správanie sa takejto zmesi. V spolupráci s hospodárskou praxou boli yvbrané potenciálne najlepšie aplikovateľné prístupy v zhodnocovaní: (i) tvorba kameniva na báze oxidov, karbidov a nitridov,

(ii) keramické vlákna pre pokročilé kompozitné materiály a (iii) pórovité materiály so tepelno izolačnými vlastnosťami. Na základe týchto zvolených smerov riešenia projektu prebieha štúdium fázových digramov v daných systémoch majoritných zložiek a výpočet vlastností tavenín (skiel). Získané poznatky budú overené experimentálnou činnosťou a celý proces bude optimalizovaný pre zvolené prístupy.

Publikácie:

HNATKO, Miroslav - SEDLÁČEK, Jaroslav - LÁZÁR, Marián. Zhodnocovanie vitrifikovanej trosky z plazmo-termického spracovania odpadov - príprava pórovitej sklo-keramickej matrice = Upgrading of vitrified slag from waste disposal by thermal plasma treatment - formation of porous glass-ceramic matrix. In Interakcie tavenín s progresívnymi anorganickými materiálmi. Bratislava: Slovenská technická univerzita v Bratislave, 2017, p. 103-112. ISBN 978-80-227-4743-1. (Interakcie tavenín s progresívnymi anorganickými materiálmi).

16.) Vývoj vodivej keramiky na báze SiC (*Development SiC based conductive ceramics*)

Zodpovedný riešiteľ:	Pavol Hvizdoš
Zodpovedný riešiteľ v organizácii SAV:	Pavol Šajgalík
Trvanie projektu:	1.10.2013 / 30.9.2017
Evidenčné číslo projektu:	APVV-0108-12
Organizácia je koordinátorom projektu:	nie
Koordinátor:	Ústav materiálového výskumu SAV
Počet spoluriešiteľských inštitúcií:	1 - Slovensko: 1
Čerpané financie:	APVV: 9028 €

Dosiahnuté výsledky:

Kompozity na báze SiC s prídavkom 20, 30 a 40% Ti a NbC, ktoré boli pripravené metódou rapid-HP, boli rozšírené o ďalšiu sériu vzoriek s prídavkom 10, 20, 30, 40 a 50 hmotnostných percent Ti a NbC. V tomto prípade boli všetky vzorky hutné, pričom vzorky s prídavkom 10 a 20 hmotnostných percent Ti a NbC boli zhutnené použitím granulovaných práškov. Voči predošlej sérii vzoriek došlo aj k skráteniu výdrže z pôvodných 30 minút na 15 minút. Mechanický tlak bol použitý na úrovni 50MPa. Vzorky boli charakterizované RTG práškovou difrakčnou analýzou, ako aj elektrónovou mikroskopiou. Na vzorkách boli zmerané mechanické vlastnosti a elektrická vodivosť. Z výsledkov vyplynulo, že došlo k signifikantnému nárastu indentačnej húževnatosti voči predošlej sérii vzoriek, avšak hodnoty elektrickej vodivosti sú rádovo 3-krát nižšie. Z analýzy mikroštruktúry vyplynulo, že došlo k jej zmene v danej sérii - fázová transformácia SiC matrice prebehla vo väčšej miere, takisto priemerná veľkosť zŕn je výrazne vyššia.

Publikácie:

FIDES, Martin - KOVALČÍKOVÁ, Alexandra - HVIZDOŠ, Pavol - BYSTRICKÝ, Roman - DŽUNDA, Róbert - BALKO, Ján - SEDLÁČEK, Jaroslav. Mechanical and tribological properties of electrically conductive SiC based cermets. In International Journal of Refractory Metals and Hard Materials, 2017, vol. 65, p. 76-82. (2.155 - IF2016). ISSN 0263-4368. Typ: ADCA

FIDES, Martin - HVIZDOŠ, Pavol - BYSTRICKÝ, Roman - KOVALČÍKOVÁ, Alexandra - SEDLÁK, Richard - SEDLÁČEK, Jaroslav - DŽUNDA, Róbert. Microstructure, fracture, electrical properties and machinability of SiC-TiNbC composites. In Journal of the European Ceramic Society, 2017, vol. 37, p. 4315-4322. (3.411 - IF2016). ISSN 0955-2219. Typ: ADCA

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. (3.411 - IF2016). ISSN 0955-2219. Typ: ADCA

FIDES, Martin - HVIZDOŠ, Pavol - DŽUNDA, Róbert - BYSTRICKÝ, Roman - SEDLÁČEK, Jaroslav. Microstructure and crack propagation of electrically conductive SiC based composites. In Materials Science Forum, 2017, vol. 891, p. 547-551. ISSN 0255-5476. Typ: ADMB

BYSTRICKÝ, Roman - SEDLÁČEK, Jaroslav - ŠKRÁTEK, Martin - ŤAPAJNA, Milan - ŠAJGALÍK, Pavol. Electrical and magnetic properties of SiC ceramics with addition of Ti and NbC. In ECerS 2017 : 15th International Conference and exhibition of the European Ceramic Society. Book of abstracts. Budapest, 9.-13.7.2017. - B.V., 2017, p. 219-220. (ECerS 2017 : International Conference and exhibition of the European Ceramic Society). Typ: AFG

HVIZDOŠ, Pavol - FIDES, Martin - KOVALČÍKOVÁ, Alexandra - BYSTRICKÝ, Roman - HNATKO, Miroslav - RUTKOWSKI, Paweł. Electrically conductive SiC based composites - development, microstructure, mechanical, electrical and tribological properties. In Polish-Slovak-Chinese seminar on ceramics : Book of abstracts. Zakopane,

13.-16.9.2017. - Krakow : Polish Ceramic Society, 2017, p. 74. ISBN 978-83-63633-97-1.(Polish-Slovak-Chinese seminar on ceramics). Typ: AFG

17.) Nanokompozitné materiály na báze organo-fosfóniových smektitov a polymérov (*Nanocomposite materials based on organo-phosphonium smectites and polymers*)

Zodpovedný riešiteľ: Peter Komadel
Trvanie projektu: 1.7.2016 / 30.6.2020
Evidenčné číslo projektu: APVV-15-0741
Organizácia je áno
koordinátorom projektu:
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 1 - Slovensko: 1
Čerpané financie: APVV: 39000 €

Dosiahnuté výsledky:

Riešenie projektu postupuje podľa schváleného harmonogramu riešenia. V roku 2017 sa riešili úlohy, ktoré patria čiastočne do prvej (07/2016 – 08/2017) a druhej (05/2017 – 07/2018) etapy. Pripravila sa séria organo-fosfóniových montmorillonitov založená na komerčne dostupných surfaktantoch alkylfosfóniových solí (alkyl-P-C16) a charakterizovala sa vybranými fyzikálno-chemickými metódami. Paralelne pokračoval aj výskum zameraný na interakcie ílových minerálov s alkylamóniovými surfaktantmi, vlastnosti ktorých sa budú porovnávať s alkylfosfóniovými. Pozornosť bola venovaná usporiadaniu organických surfaktantov v medzivrstviach montmorillonitu, ktorá má vplyv na vlastnosti organoílov, napr. na expanziu medzivrstvového priestoru ílového minerálu. Splnili sa aj plánované ciele v oblasti syntézy nových, komerčne nedostupných alkylfosfóniových solí s rôznou dĺžkou alkylových reťazcov. Súčasne sa s určitým predstihom začali experimenty týkajúce sa sledovania vlastností polymérno-ílových nanokompozitov s plnivami modifikovanými alkylamóniovými kationmi, pričom získané výsledky sa použijú pre porovnanie s vlastnosťami kompozitov s fosfóniovými modifikáciami organoílov. Študovala sa aj interakcia ílových minerálov s organickými fluorescenčnými farbivami. Pomocou DFT metódy sa uskutočnili výpočty intarkalačných energií zamerané na porovnanie stability montmorillonitov a beidelitov modifikovaných tetrabutylfosfóniovým kationom. Táto metóda umožňuje opísať väzbové a štruktúrne pomery v látkach vrátane jemných štruktúrnych trendov, vibračných módo, ako aj mechanických vlastností týchto materiálov.

PÁLKOVÁ, H. – ZIMOWSKA, M. – JANKOVIČ, Ľ. – SULIKOWSKI, B. – SERWICKA, E.M. – MADEJOVÁ, J. 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). ISSN 0169-1317. Typ: ADCA
 BIZOVSKÁ, V. - JANKOVIČ, Ľ. - MADEJOVÁ, J. Montmorillonite modified with less-traditional surfactants from the series of octylammonium-based cations: Structural characterization and hydration properties. Odoslané v 2017 do *Applied Clay Science*, (3.101 – IF2016).
 SEDNIČKOVÁ, M. – JOCHEC MOŠKOVÁ, D. – JANIGOVÁ, I. – KRONEK, J. – JANKOVIČ, Ľ. – ŠLOUF, M. – CHODÁK, I. Properties of natural rubber composites with structurally different clay intercalable surfactants. In *Journal of Polymer Research*, 2017, vol. 24, art. no. 105. (1.615 – IF2016). ISSN 1022-9760. Typ: ADCA
 JOCHEC MOŠKOVÁ D - JANIGOVÁ, I. - Nógellová, Z. - Sedničková, M. - JANKOVIČ, Ľ. - KOMADEL, P. - ŠLOUF, M. – CHODÁK, I. Characterization of filler reinforcing structure in polymer – clay nanocomposites and its prediction by rheological measurements. Odoslané v 2017 do *POLYMER TESTING*, (IF2016=2.464)
 SCHOLTZOVÁ, E. – TUNEGA, D. DFT study of stability of the tetrabutylphosphonium and tetrabutylammonium montmorillonites. Odoslané v 2017 do *Clay Minerals* (IF2016=1.052)
 CZÍMEROVÁ, A. – ČEKLOVSKÝ, A. Resonance energy transfer between rhodamine dyes in saponite thin films: a step towards novel photofunctional nanohybrids. In *Clay Minerals*, 2017, vol. 52, p. 263-273. (1.052 – IF2016). ISSN 0009-8558. Typ: ADCA
 BELUŠÁKOVÁ, S. – MARTÍNEZ-MARTÍNEZ, V. – LOPEZ ARBELOA, I. – BUJDÁK, J. 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. Typ: ADCA
 CZÍMEROVÁ, A. – SAS, S. – ČEKLOVSKÝ, A. Unique solvatochromism of cyanine/saponite hybrid systems. In *Applied Clay Science*, 2017, vol. 141, p. 198-203. (3.101 – IF2016). ISSN 0169-1317. Typ: ADCA
 CZÍMEROVÁ, A. - ČEKLOVSKÝ, A. Fluorescence energy transfer between dye cations in saponite: from colloids to Langmuir-Blodgett films. Odoslané do *Chemical Papers* (IF2016=1.258)
 SAS, S. – DANKO, M. – BIZOVSKÁ, V. – LANG, K. – BUJDÁK, J. Highly luminescent hybrid materials based on smectites with polyethylene glycol modified with rhodamine fluorophore. In *Applied Clay Science*, 2017, vol. 138, p. 25-33. (3.101 – IF2016). ISSN 0169-1317. Typ: ADCA

18.) Fotoluminescenčné keramické materiály na báze oxynitridov kremíka (*Silicon oxynitride-based photoluminescent ceramic materials*)

Zodpovedný riešiteľ:	Zoltán Lenčoš
Trvanie projektu:	1.7.2015 / 30.6.2019
Evidenčné číslo projektu:	APVV-14-0385
Organizácia je koordinátorom projektu:	áno
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	2 - Slovensko: 2
Čerpané financie:	APVV: 35679 €

Dosiahnuté výsledky:

Luminofoxy na báze LaSi_3N_5 a dopované lantanoidmi ($\text{Ln} = \text{Ce}, \text{Er}, \text{Yb}$) boli pripravené zo zmesí $\text{LaSi}_3\text{N}_5/\text{LnF}_3$ a $\text{LaSi}_3\text{N}_5/\text{Ln}_2\text{O}_3$ žiňaním pri 1600 °C po dobu 3 h v pretlaku dusíka 2 MPa. Luminofoxy dopované fluoridmi vykazujú pomerne ostré/úzke emisné píky s maximom 546 nm pre CeF_3 -dopovaný materiál, pri 397 nm a 468 nm pre ErF_3 a pri 483 nm pre YbF_3 dopovaný LaSi_3N_5 luminofoxy. V prípade luminofofov LaSi_3N_5 dopovaných oxidmi lantanoidov boli namerané výrazne širšie emisné píky (pri 510 – 625 nm pre CeO_2 dopovaný materiál, 370 – 600 nm pre Er_2O_3 , a 440 – 600 nm pre Yb_2O_3 dopovaný materiál). Poloha maxim bola približne rovnaká, ako u luminofofov dopovaných fluoridmi lantanoidov.

Pri príprave luminofofov na báze O'-sialonu ($\text{Si}_{2-x}\text{Al}_x\text{O}_{1+x}\text{N}_{2-x}$, tzn. tuhý roztok $\text{Si}_2\text{N}_2\text{O}$ a Al_2O_3) boli študované dva spôsoby: i) príprava O'-sialonu reakciami v tuhej fáze zo zmesi $\text{Si}_3\text{N}_4 + \text{SiO}_2 + \text{Al}_2\text{O}_3$ a ii) zo zmesi Si_3N_4 a SiAlOC polymérneho prekursoru. Výsledky ukázali, že príprava O'- SiAlON u reakciami v tuhej fáze je veľmi pomalá a po syntéze prášku pri 1800°C po dobu 2 hodín v pretlaku dusíka (1,5 MPa) produkt pozostával z majoritného Si_3N_4 , $\text{Si}_2\text{N}_2\text{O}$ (20%), minoritného Al_2O_3 a amorfného SiO_2 . Druhú spôsob syntézy je efektívnejší, zo zmesi Si_3N_4 a SiAlOC sa podarilo pripraviť O'- SiAlON pri nižších teplotách (1750°C) a kratších časoch (15 min). Na zabudovanie dopantu (Eu) do štruktúry O'- SiAlON u bolo nutné vzorky ďalej žiňat pri 1650°C po dobu 2 hodín. Luminofoxy O'- SiAlON:Eu emitoval žiarenie v žltej oblasti viditeľného svetla. Intenzita emitovaného žiarenia bola zvýšená dôkladným odstránením (výpalom) uhlíka z SiAlOC polymérneho prekursoru (800°C, 1 h na vzduchu) pred samotným žiňaním, lebo zostatkový uhlík v luminofofe znižoval intenzitu emitovaného žiarenia.

Namiesto SiAlOC prekursorov boli použité aj prekursor SiHfOC a SiLuOC . Luminofoxy boli pripravené za rovnakých podmienok, ako v prípade SiAlOC prekursorov. Fotoluminiscenčné merania ukázali, že SiHfON:Eu emituje v zeleno-žltej oblasti a SiLuON:Eu emituje v zelenej oblasti viditeľného svetla. Emisie však mali nižšiu intenzitu v porovnaní s luminofofmami na báze SiAlON:Eu , lebo SiHfON a SiLuON nevytvorili tuhý roztok s Si_3N_4 .

Metódou MOCVD boli pripravené tenké fotoluminiscenčné vrstvy (20-25 nm) YAG:Ce na kremenných sklíčkach. Luminofoxy YAG:Ce emitoval žiarenie v zelenej oblasti viditeľného svetla. Študoval sa aj vplyv žiňania vzoriek v rôznych atmosférach (O_2 , N_2 , N_2+H_2) na farbu emitovaného žiarenia. Redukčná atmosféra (H_2) spôsobila červený posuv emitovaného žiarenia. Po vystavení luminofofov vzdušnej vlhkosti po dlhšiu dobu (3-4 týždne) došlo k degradácii ich vlastností. Tento problém sa podarilo odstrániť nanosením 10 nm hrubej Al_2O_3 ochrannnej vrstvičky na YAG vrstvu. Vrstevnatý ($\text{YAG:Ce}/\text{Al}_2\text{O}_3$) luminofoxy má veľmi dobrú stabilitu.

19.) Genéza perlitu a inovatívne prístupy pri jeho ťažbe a spracovaní (*Perlite genesis and innovative approaches to its exploitation and processing*)

Zodpovedný riešiteľ:	Jana Madejová
Trvanie projektu:	1.10.2013 / 30.9.2017
Evidenčné číslo projektu:	APVV-0339-12
Organizácia je koordinátorom projektu:	nie
Koordinátor:	Prírodovedecká fakulta UK
Počet spoluriešiteľských inštitúcií:	2 - Slovensko: 2
Čerpané financie:	APVV: 6405 €

Dosiahnuté výsledky:

V roku 2017 v súlade s harmonogramom projektu prebiehala Záverečná etapa projektu, ktorá zo strany ústavu a spoluriešiteľa projektu zahŕňala sumarizáciu výsledkov o množstve, forme a rýchlosti uvoľňovania vody zo študovaných perlitov z ložísk Lehôtka pod Brehmi a Jastrabá. Obsah vody je jeden z najdôležitejších parametrov kvality perlitu. Jednotlivé vzorky perlitov sa vzájomne odlišovali obsahom vody (v priemere to bolo pre jednotlivé typy: 4, 3,5 a 5,2 hm. %). Pomocou IČ spektroskopie v blízkej oblasti sa sledovalo uvoľňovanie vody v závislosti od teploty. Okrem toho sa podarilo pripraviť metodiku na kvantitatívne určovanie množstva vody pomocou IČ spektroskopie a štandardu. Vypracoval sa inovatívny postup na kvantitatívne určenie množstva vody pomocou IČ spektroskopie a vloženého štandardu. Stanovenie množstva vody na základe IČ spektier sa uskutočnilo rôznymi spôsobmi a získané výsledky sa porovnávali s výsledkami získanými z termickej analýzy a gravimetrických experimentov. Ako štandardy sa vybrali dva materiály, ktoré neobsahujú vodu a navyše vykazujú k nej veľmi nízku afinitu: hexadecyltrimetylamóniový bromid (HDTMA) resp. mastenec. Obe látky majú intenzívny absorpčný pás, na ktorý sa dajú normovať spektrá a nevykazujú žiadne pásy vody, ktoré by sa prekrývali s pásmi vody perlite. Po normalizácii spektier, zmeraní plochy kombinačnej vibrácie vody v perlite a porovnaní týchto hodnôt s obsahom vody z TG analýzy sa pri oboch štandardoch získala dobrá korelácia pre rôzne metódy stanovenia vody.

20.) Vývoj nových teoretických nástrojov pre predikciu a interpretáciu EPR a NMR parametrov (Developing new theoretical tools for prediction and interpretation of EPR and NMR parameters)

Zodpovedný riešiteľ: Vladimír Malkin
Trvanie projektu: 1.7.2016 / 30.6.2020
Evidenčné číslo projektu: APVV-15-0726
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 1 - Slovensko: 1
Čerpané financie: APVV: 35860 €

Dosiahnuté výsledky:

BÜCHEL, Gabriel E. - KOSSATZ, Susanne - SADIQUE, Ahmad - RAPTA, Peter - ZALIBERA, Michal - BUČINSKÝ, Lukáš - KOMOROVSKÝ, Stanislav - TELSER, Joshua - EPPINGER, Jörg - REINER, Thomas - ARION, Vladimír. cis-Tetrachlorido-bis(indazole)osmium(IV) and its osmium(III) analogues: paving the way towards the cis-isomer of the ruthenium anticancer drugs KP1019 and/or NKP1339. In Dalton Transactions, 2017, vol. 46, no. 35, p. 11925-11941. (4.029 - IF2016).

MALKIN, Vladimír - MALKINA, Olga - ZHIDOMIROV, Georgy M. Visualization of electron paramagnetic resonance hyperfine structure coupling pathways. In Journal of Physical Chemistry A.Molecules, spectroscopy, kinetics, environment, and general theory, 2017, vol. 121, no. 18, p. 3580-3587. (2.847 - IF2016).

21.) Vlastnosti nových progresívnych konštrukčných materiálov v agresívnom prostredí roztavených solí (The behaviour of new progressive construction materials in aggressive environment of molten salts)

Zodpovedný riešiteľ: František Šimko
Trvanie projektu: 1.7.2016 / 30.6.2020
Evidenčné číslo projektu: APVV-15-0738
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 1 - Slovensko: 1
Čerpané financie: APVV: 40000 €

Dosiahnuté výsledky:

Projekt je zameraný na komplexný výskum koróznych procesov pokročilých konštrukčných materiálov, prebiehajúcich v agresívnych roztavených fluoridových soliach. Objektami výskumu sú špeciálne keramické materiály na báze SiC, pre vysokoteplotné aplikácie v agresívnom prostredí roztavených fluoridových tavenín. Uskutočnili sa dlhotrvajúce korózne experimenty daných materiálov v eutektickej zmesi binárnych zlúčenín (LiF-NaF-KF)_{eut.} pri teplote 700oC. Korózne produkty boli analyzované pomocou XRD, IR, SEM-EDX a EBSD analytických metód. Pred experimentami sa realizovali práce na prípravu experimentálnych zariadení, slúžiacich na statické, dlhodobé, korózne testy.

Publikácie:

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. (6.455 - IF2016). ISSN 1040-8436.

KONTRÍK, Martin - ŠIMKO, František - JANIČKOVIČ, Dušan - NOSKO, Martin - KORENKO, Michal - BOČA, Miroslav. Corrosion resistance of inert anode material with different crystal structure in molten low-temperature fluoride salt. In Preparation of ceramic materials : Proceedings of the 12th international conference. Jahodná, 13.-15.6.2017. Ed. B. Plešingerová et al. Košice: Technical University, 2017, p. 164-165. ISBN 978-80-553-3160-7. (Preparation of ceramic materials : international conference).

Programy: SASPRO**22.) Vlastnosti materiálov po vysokoteplotných koróziách v roztopených soliach** (*High-temperature properties of materials corrosion in molten salts*)

Zodpovedný riešiteľ: Miroslav Boča
Trvanie projektu: 5.11.2015 / 4.11.2018
Evidenčné číslo projektu: 1119/02/02
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 58687 €

Dosiahnuté výsledky:

Projekt začal literárnou rešeršou, čo malo za úlohu pomôcť pochopiť aktuálnu problematiku vo svete a zároveň pomôcť pri písaní prehľadného článku týkajúceho sa problematiky. Od začatia projektu sa skúmali korózne charakteristiky spomínaných zliatin v prostrediach roztavených fluoridov (LiF-NaF-KF) pri teplote 680 °C a roztavených chloridov (NaCl-KCl, NaCl-KCl-UCI₄ & NaCl-KCl-ZrCl₄) pri teplote 750 °C. Experimenty boli uskutočnené na daných teplotách s časmi výdrží od 6 do 100 hodín, kvôli pochopeniu korózneho správania sa testovaných zliatin pri zvolených intervaloch. Z hľadiska korózie superzliatin sa ukázalo, že pri koróznom čase do sto hodín sú stále významné len počiatočné fázy korózie. Predchádzajúce štúdie poukázali, že práve tieto sú najviac kritickými. Keďže roztavené soli sa chovajú ako elektrolyt, boli uskutočnené aj elektrochemické osemhodinové merania. Na objasnenie morfológie povrchu a rezov korodovaných vzoriek boli použité techniky mikroštruktúrálnej charakterizácie, kde sa taktiež vyhodnocovala hĺbka korózie. Naše experimenty poskytujú detailný pohľad na počiatočnú fázu korózie testovaných zliatin s použitím rôznych korózných prostredí.

Publikácie:

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. (6.455 - IF2016). ISSN 1040-8436.

Niketan Patel, Viliam Pavlík; Blanka Kubíková; Martin Nosko; Vladimír Danielik; Miroslav Boča. Corrosion behavior of Ni-based superalloys in molten FLiNaK salts. Zasláné do Materials and Corrosion.

PAVLÍK, Viliam - PATEL, Niketan Sarabhai - BOČA, Miroslav. Interakcia zliatiny Incoloy 800 HT a taveniny (LiF-NaF-KF)Eut. za prítomnosti chromitých solí = Interaction between Incoloy 800HT alloy and molten mixture (LiF-NaF-KF)Eut. with additions of chromic salts. In 59. medzinárodná galvanická konferencia : zborník prednášok. Ed. Vladimír Danielik ; recenzenti: Pavel Fellner, Ján Híveš, Matilda Zemanová. - Bratislava : Slovenská technická univerzita, 2017, s. 19-25. ISBN 978-80-227-4705-9. (Medzinárodná galvanická konferencia)

23.) Zviditeľniť relativistickú kvantovú chémiu: Relativistické paramagnetické NMR (*Moving relativistic quantum chemistry out of the shadow: Relativistic paramagnetic NMR*)

Zodpovedný riešiteľ: Vladimír Malkin
Trvanie projektu: 1.10.2016 / 31.12.2018
Evidenčné číslo projektu: 1536/03/02
Organizácia je koordinátorom projektu: áno

Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 56654 €

Dosiahnuté výsledky:

4cPNMR project má päť hlavných cieľov. V každom smere bol dosiahnutý čiastkový úspech zodpovedajúci fáze v ktorej sa project nachádza.

1. Vývoj a implementácia relativistickej metódy určenej na výpočet nízko ležiacich excitovaných stavov:
 V prvej časti projektu 4cPNMR sme vyvinuli a implementovali do programu ReSpect relativistickú štvorkomponentnú časovo závislú teóriu funkcionálu hustoty (4k-ČZTFH) pre referenčné systémy s uzavretým aj otvoreným obalom. Ide o významný výsledok, keďže doteraz vedecká komunita považovala implementovanie metódy ČZTFH pre systémy s otvoreným obalom za príliš náročné alebo priam nemožné. Dve publikácie popisujúce teóriu a implementáciu metódy 4k-ČZTFH sú v štádiu prípravy.

2. Vývoj a implementácia metód určených na výpočet pNMR na systémoch s vyššou ako dvojistou degeneráciou základného stavu:

Zhodou okolností sme v rámci projektu 4cPNMR objavili nové kvantové číslo pre relativistický mnoho-elektrónový systém [Phys. Rev. A 94, 052104 (2016)]. Nové kvantové číslo má potenciál nahradiť spinovú symetriu v relativistickej doméne čím nepriamo pomôže aj pri riešení 4cPNMR projektu. Podľa nášho názoru je tento objav najvýznamnejší teoretický výsledok projektu 4cPNMR, hoci nebol priamou súčasťou projektového plánu:

3. Implementácia moderných programovacích techník určených na zvýšenie efektívnosti kódu, čo umožní aplikovať vyvinuté metódy na systémoch obsahujúcich až 200 atómov:

V prvej fáze 4cPNMR projektu sme implementovali MPI paralelizáciu TFH jadier a Cauchy-Schwartzovej nerovnosti pre štvorcentrové integrály.

4. Zverejnenie kódu na webovej stránke ReSpect vrátane manuálov, návodov a predkompilovaných statických a dynamických binárnych súborov:

Vykonalí sme výrazné zlepšenia vstupnej štruktúry dát a spúšťacích skriptov a pracujeme na novej webovej stránke ReSpect programu vrátane novej príručky a návodov.

5. Uverejnenie teoretických článkov "dôkaz koncepcie" a aplikácia vyvinutých metód v spolupráci s našimi zahraničnými partnermi:

Aj keď bola aplikácia vyvinutých metód naplánovaná až na ďalšiu fázu projektu naskytla sa nám možnosť spolupráce už počas prvého roka 4cPNMR projektu.

- Vývoj nových protirakovinových liekov (široká medzinárodná spolupráca skupín v USA, Rakúsku, Saudskej Arábii a na Slovensku) [Dalton Trans. 46, 11925 (2017)].

• Vysvetlenie zmeny spin-orbitálneho NMR posunu ľahkých atómov v blízkosti ťažkého atómu na základe poruchovej teórie [J. Chem. Theory Comput. 13, 3586 (2017)].

• Štúdium ligandových hyperjemných pNMR efektov [Online, Inorg. Chem. (2017)].

Výsledky boli ďalej prezentované nasledovne:

-dve pozvané prednášky na medzinárodných konferenciách: "Xth Workshop on Modern Methods in Quantum Chemistry (Mariapfarr, Rakúsko, 6. 3. 2017)" a "12th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics (REHE) (Marburg, Nemecko, 4. 9. 2017)".

-dva semináre u našich zahraničných partnerov: "Helmholtz-Zentrum Dresden-Rossendorf: Chemistry of the f-elements (Dražďany, Nemecko, 6. 6. 2017)" a "Technische Universität Berlin, Institut für Chemie (Berlín, Nemecko, 8. 9. 2017)".

24.) Transparentné luminescentné oxinitridy (*Transparent luminescent oxynitrides*)

Zodpovedný riešiteľ: Pavol Šajgalík
Trvanie projektu: 1.1.2016 / 31.12.2018
Evidenčné číslo projektu: 1329/03/03
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0

Čerpané financie:

SAV: 79921 €

Dosiahnuté výsledky:

Optimalizáciou reologických vlastností a stability suspenzií obsahujúcich spinel (MgAl_2O_4) a následným vymrazovaním v kvapalnom dusíku a odsublímovaním ľadu sa podarilo pripraviť granule MgAl_2O_4 s definovaným priemerom. Granulovaný prášok má lepšiu zabiehavosť do lisovacej formy, čím sa dosiahla vyššia hustota výliskov a následne aj nižšia pórovitosť spekaného materiálu. Boli optimalizované podmienky dvojstupňového spekania keramických vzoriek, konkrétne beztlakové spekanie v rýchlom žiarovom lise (rapid hot-pressing) a následné dospekanie vzoriek v izostatickom žiarovom lise (HIP – hot isostatic press). Po optimalizácii podmienok lisovania a spekania vzoriek dosiahla reálna in-line optická priepustnosť (RIT) transparentných MgAl_2O_4 vzoriek ~90% teoretickej hodnoty. Doposiaľ publikované hodnoty RIT pre MgAl_2O_4 sú na úrovni 85%.

Na prípravu luminoforov na báze MgAlONu (tuhý roztok v sústave $\text{MgO-Al}_2\text{O}_3\text{-AlN}$) bol študovaný vplyv východiskového zloženia prášku, tzn. pomeru $\text{MgO:Al}_2\text{O}_3\text{:AlN}$ z oblasti tuhého roztoku na morfológiu častíc MgAlON . Po štúdiu siedmych rôznych zložení bolo zistené, že morfológia častíc MgAlONu syntetizovaných z oblasti bohatšej na kyslík (menej dusíka) pozostávala zo silne aglomerovaných častíc s veľkosťou $d_{50} > 10 \mu\text{m}$, kým prášky syntetizované z práškov s nižším obsahom kyslíka (vyšším obsahom dusíka) boli menej aglomerované a veľkosť častíc bola menšia ($d_{50} \leq 1 \mu\text{m}$). Mechanizmus rastu kryštálov zodpovedal Kosselovmu modelu.

Pri príprave luminoforov na báze O'-sialonu ($\text{Si}_{2-x}\text{Al}_x\text{O}_{1+x}\text{N}_{2-x}$, tzn. tuhý roztok $\text{Si}_2\text{N}_2\text{O}$ a Al_2O_3) boli študované dva spôsoby: i) príprava O'-sialonu reakciami v tuhej fáze zo zmesi $\text{Si}_3\text{N}_4 + \text{SiO}_2 + \text{Al}_2\text{O}_3$ a ii) zo zmesi Si_3N_4 a SiAlOC polymérneho prekurzoru. Výsledky ukázali, že príprava O'-sialonu reakciami v tuhej fáze je veľmi pomalá a po syntéze prášku pri 1800°C po dobu 2 hodín v pretlaku dusíka (1,5 MPa) produkt pozostával z majoritného Si_3N_4 , $\text{Si}_2\text{N}_2\text{O}$ (20%), minoritného Al_2O_3 a amorfného SiO_2 . Druhú spôsob syntézy je efektívnejší, zo zmesi Si_3N_4 a SiAlOC sa podarilo pripraviť O'-sialon pri nižších teplotách (1750°C) a kratších časoch (15 min). Na zabudovanie dopantu (Eu) do štruktúry O'-sialonu bolo nutné vzorky ďalej žihať pri 1650°C po dobu 2 hodín. Luminofor O'-sialon:Eu emitoval žiarenie v žltej oblasti viditeľného svetla. Intenzita emitovaného žiarenia bola zvýšená dôkladným odstránením (výpalom) uhlíka z SiAlOC polymérneho prekurzoru (800°C , 1 h na vzduchu) pred samotným žihaním, lebo zostatkový uhlík v luminofore znižoval intenzitu emitovaného žiarenia.

Publikácie:

M. Radwan, Z. Lenčoš, P. Šajgalík: Morphology of MgAlON powders synthesized by solid-state reaction, effect of composition and mechanism of crystal growth. *J. Eur. Ceram. Soc.*, zaslané do tlače.

Príloha C - Publikačná činnosť organizácie (generovaná z ARL)**ABA Štúdie charakteru vedeckej monografie v časopisoch a zborníkoch vydané v zahraničných vydavateľstvách**

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ABC Kapitoly vo vedeckých monografiách vydané v zahraničných vydavateľstvách

- ABC01 GATES, W.P. - PETIT, Sabine - MADEJOVÁ, Jana. Applications of NIR/MIR to determine site occupancy 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.
- ABC02 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. ISSN 1572-4352.
- ABC03 MADEJOVÁ, Jana - PÁLKOVÁ, Helena. NIR contribution to the study of modified clay minerals. In Infrared and Raman spectroscopies of clay minerals. - Netherlands : Elsevier, 2017, p. 447-481. ISBN 978-0-08-100355-8. ISSN 1572-4352.
- ABC04 MACHÁČEK, Jan - CHROMČÍKOVÁ, Mária - LIŠKA, Marek. Parameterization and validation of thermochemical models of glass by advanced statistical analysis of spectral data : Chapter 12. In Thermal physics and thermal analysis : From macro to micro, highlighting thermodynamics, kinetics and nanomaterials. - Switzerland : Springer International Publishing AG, 2017, p. 257-278. ISBN 978-3-319-45897-7. ISSN 1571-3105.
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- ADCA02 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). (2017 - Current Contents). ISSN 1932-7447.
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- ADCA05 BROCLAWIK, Ewa - GÓRA-MAREK, Kinga - RADOŃ, Mariusz - BUČKO, Tomáš - STEPNIEWSKI, Adam. The dependence on ammonia pretreatment of N-O activation by Co(II) sites in zeolites: a DFT and ab initio molecular dynamics study. In Journal of

- molecular modeling, 2017, vol. 23, no. 5, p. 160-1-160-13. (1.425 - IF2016). (2017 - Current Contents). ISSN 1610-2940.
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- ADCA07 BÜCHEL, Gabriel E. - KOSSATZ, Susanne - SADIQUE, Ahmad - RAPTA, Peter - ZALIBERA, Michal - BUČINSKÝ, Lukáš - KOMOROVSKÝ, Stanislav - TELSER, Joshua - EPPINGER, Jörg - REINER, Thomas - ARION, Vladimír.
cis-Tetrachlorido-bis(indazole)osmium(IV) and its osmium(III) analogues: paving the way towards the cis-isomer of the ruthenium anticancer drugs KP1019 and/or NKP1339. In Dalton Transactions, 2017, vol. 46, no. 35, p. 11925-11941. (4.029 - IF2016). (2017 - Current Contents). ISSN 1477-9226.
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- ADCA10 CZÍMEROVÁ, Adriana - ČEKLOVSKÝ, Alexander. Resonance energy transfer between rhodamine dyes in saponite thin films: a step towards novel photofunctional nanohybrids. In Clay Minerals, 2017, vol. 52, p. 263-273. (1.052 - IF2016). (2017 - Current Contents). ISSN 0009-8558.
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- ADCA14 FIDES, Martin - KOVALČÍKOVÁ, Alexandra - HVIŽDOŠ, Pavol - BYSTRICKÝ, Roman - DŽUNDA, Róbert - BALKO, Ján - SEDLÁČEK, Jaroslav. Mechanical and tribological properties of electrically conductive SiC based cermets. In International Journal of Refractory Metals and Hard Materials, 2017, vol. 65, p. 76-82. (2.155 - IF2016). (2017 - Current Contents). ISSN 0263-4368.
- ADCA15 FIDES, Martin - HVIŽDOŠ, Pavol - BYSTRICKÝ, Roman - KOVALČÍKOVÁ, Alexandra - SEDLÁK, Richard - SEDLÁČEK, Jaroslav - DŽUNDA, Róbert. Microstructure, fracture, electrical properties and machinability of SiC-TiNbC composites. In Journal of the European Ceramic Society, 2017, vol. 37, p. 4315-4322. (3.454 - IF2016). (2017 - Current Contents). ISSN 0955-2219.
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BDB Heslá v odborných terminologických slovníkoch a encyklopédiách vydaných v domácich vydavateľstvách

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- ADEB01 GALUSEK, Dušan - KIDO, Ladislav - PÁNEK, Zdeněk - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol - RILEY, F.L. The influence of sintering additives on the fracture behaviour and wear of liquid-phase sintered polycrystalline alumina. In Key Engineering Materials, 2002, vol. 223, p. 227-232. (2002 - SCOPUS).

Citácie:

1. [1.1] HU, Dezhi - LI, Zhihong - ZHU, Yumei. Effect of ZnF₂-TiO₂-SiO₂ additions on the two-step sintering behavior and mechanical properties of sol-gel derived corundum abrasive. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2016, vol. 42, no. 6, pp. 7373., WOS

- ADEB02 GALUSEK, Dušan - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol - RIEDEL, Ralf. Thermal analysis study of polymer-to-ceramic conversion of organosilicon precursors. In Journal of Mining and Metallurgy : Section B: Metallurgy, 2008, vol. 44, no. 1, p. 35-38. ISSN 1450-5339.

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1. [1.1] CARNI, D. L. - GRIMALDI, D. - SCIAMMARELLA, P. F. - NASTRO, A. - LAMONACA, F. - VASILE, M. Measurement technique for the healthy and carious teeth based on thermal analysis. In 2016 IEEE INTERNATIONAL SYMPOSIUM ON MEDICAL MEASUREMENTS AND APPLICATIONS (MEMEA), 2016, vol., no., pp. 171-175., WOS

- ADEB03 HNATKO, Miroslav - ŠAJGALÍK, Pavol - LENČEŠ, Zoltán - MONTEVERDE, F. - DUSZA, Ján - WARBIHLER, P. - HOFFER, F. Low cost SiC/Si₃N₄ nanocomposites. In Key Engineering Materials, 2002, vol. 206-213, p. 1061-1064. (2002 - SCOPUS).

Citácie:

1. [1.1] CHAROO, M. S. - WANI, M. F. Friction and wear properties of nano-Si₃N₄/nano-SiC composite under nanolubricated conditions. In JOURNAL OF ADVANCED CERAMICS. ISSN 2226-4108, 2016, vol. 5, no. 2, pp. 145., WOS

- ADEB04 LENČEŠ, Zoltán - HIRAO, Kiyoshi - ŠAJGALÍK, Pavol - HOFFMANN, M.J. Thermodynamic and dielectric properties of MgSiN₂ ceramics. In Key Engineering Materials, 2006, vol. 317-318, p. 857-860. (0.224 - IF2005). (2006 - SCOPUS). ISSN 1013-9826.

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1. [1.1] ARAB, Fahima - SAHRAOUI, F. Ali - HADDADI, Khelifa - BOUHEMADOU, Abdelmadjid - LOUAIL, Layachi. Phase stability, mechanical and thermodynamic properties of orthorhombic and trigonal MgSiN₂: an ab initio study. In PHASE TRANSITIONS. ISSN 0141-1594, 2016, vol. 89, no. 5, pp. 480., WOS

ADMB Vedecké práce v zahraničných neimpaktovaných časopisoch registrovaných v databázach Web of Science alebo SCOPUS

- ADMB01 BALOG, Miroslav - ŠAJGALÍK, Pavol - LENČEŠ, Zoltán - HNATKO, Miroslav - KEČKÉŠ, Jozef. Hardness limits of SiC and Si₃N₄ ceramic materials. In Key Engineering Materials, 2005, vol. 287, p. 311-316. (0.278 - IF2004). (2005 - SCOPUS). ISSN 1013-9826.

Citácie:

1. [1.1] EOM, Jung-Hye - SEO, Yu-Kwang - KIM, Young-Wook. Mechanical and Thermal Properties of Pressureless Sintered Silicon Carbide Ceramics with Alumina-Yttria-Calcia. In JOURNAL OF THE AMERICAN CERAMIC SOCIETY. ISSN 0002-7820, 2016, vol. 99, no. 5, pp. 1735-1741., WOS

- ADMB02 BALOG, Miroslav - ŠAJGALÍK, Pavol - LENČEŠ, Zoltán - KEČKÉŠ, Jozef - HUANG, J.-L. Liquid phase sintering of SiC with AlN and rare-earth oxide additives. In Ceramic Transactions : Silicon-Based Structural Ceramics for the New Millennium, 2003, vol. 142, p. 191-202.

Citácie:

1. [1.1] LIANG, Hanqin - YAO, Xiumin - HUANG, Zhengren - ZENG, Yuping - SU, Bizhe. Effect of sintering techniques on the microstructure of liquid-phase-sintered SiC ceramics. In JOURNAL OF THE EUROPEAN CERAMIC SOCIETY. ISSN 0955-2219, 2016, vol. 36, no. 8, pp. 1863-1871., WOS

- ADMB03 KOMADEL, Peter - MADEJOVÁ, Jana - VALÚCHOVÁ, Jana - JANEK, Marián - BUJDÁK, Juraj. Fixation of Li⁺ cations in montmorillonite upon heating. In Solid State

Phenomena, 2003, vol. 90-91, p. 497-502. (2003 - Current Contents). ISSN 1012-0394.(Solid State Chemistry V : 5th International Conference on Solid State Chemistry).

Citácie:

1. [1.1] KRZYZANOWSKI, Andrzej - ZAREBSKA, Katarzyna - BARAN, Pawel. Effect of Li⁺ stabilization on smectite intercalate properties. In COLLOID JOURNAL. ISSN 1061-933X, 2016, vol. 78, no. 3, pp. 331., WOS

***AEC Vedecké práce v zahraničných recenzovaných vedeckých zborníkoch, monografiách**

AEC01 SEDLÁČEK, Jaroslav - GALUSEK, Dušan - ŠVANČÁREK, Peter - BROWN, Andy - BRYDSON, R. Alumina-carbon composites with high hardness. In EURO CERAMICS VIII. PTS 1-3. Eds. H. Mandal, L. Ovecoglu. - 2004, p. 841-844. ISBN 0-87849-946-6. ISSN 1013-9826.

Citácie:

1. [1.1] KRISHNAMURITHY, Genasan - YAHYA, Noor Azlin - MEHRALI, Mehdi - MEHRALI, Mohammad - MOHAN, Saktiswaren - MURALI, Malliga Raman - RAGHAVENDRAN, Hanumantha Rao Balaji - KAMARUL, Tunku. Effects of carbon doping on the microstructural, micro/nano-mechanical, and mesenchymal stromal cells biocompatibility and osteogenic differentiation properties of alumina. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2016, vol. 42, no. 16, pp. 18247-18256., WOS

Príloha D - Údaje o pedagogickej činnosti organizácieSemestrálne prednášky:

prof. RNDr. Jozef Noga, DrSc.

Názov semestr. predmetu: General and Inorganic Chemistry

Počet hodín za semester: 60

Názov katedry a vysokej školy: Uniwersytet Śląski Katowice, Poľsko, Instytut Chemii

Ing. František Šimko, PhD.

Názov semestr. predmetu: Anorganická chémia 2

Počet hodín za semester: 4

Názov katedry a vysokej školy: Prírodovedecká fakulta UK, Katedra anorganickej chémie

Semestrálne cvičenia:

Mgr. Silvia Belušáková, PhD.

Názov semestr. predmetu: Fyzikálna chémia - laboratórne cvičenia

Počet hodín za semester: 117

Názov katedry a vysokej školy: Prírodovedecká fakulta UK, Katedra fyzikálnej chémie

Mgr. Valéria Bizovská, PhD.

Názov semestr. predmetu: Odborná prax

Počet hodín za semester: 50

Názov katedry a vysokej školy: Prírodovedecká fakulta UK, Katedra anorganickej chémie

Ing. Helena Pálková, PhD.

Názov semestr. predmetu: Špeciálne metódy výskumu nerúd pre študentov 4. ročníka

Počet hodín za semester: 2

Názov katedry a vysokej školy: Prírodovedecká fakulta UK, Katedra ložiskovej geológie

Semináre:

Mgr. Silvia Belušáková, PhD.

Názov semestr. predmetu: Physical Chemistry

Počet hodín za semester: 20

Názov katedry a vysokej školy: Prírodovedecká fakulta UK, Katedra fyzikálnej chémie

Mgr. Stanislav Kedžuch, PhD.

Názov semestr. predmetu: Výpočtový seminár II

Počet hodín za semester: 48

Názov katedry a vysokej školy: Prírodovedecká fakulta UK, Katedra anorganickej chémie

Terénne cvičenia:Individuálne prednášky:

doc. Ing. Miroslav Hnatko, PhD.

Názov semestr. predmetu: Príprava a vlastnosti pokročilej keramiky II.

Počet hodín za semester: 3

Názov katedry a vysokej školy: Fakulta chemickej a potravinárskej technológie STU, Ústav anorganickej chémie, technológie a materiálov

Mgr. Stanislav Komorovský, PhD.

Názov semestr. predmetu: A new quantum number for the many-electron Dirac–Coulomb Hamiltonian

Počet hodín za semester: 2

Názov katedry a vysokej školy: Fakulta matematiky, fyziky a informatiky UK, Katedra teoretickej fyziky a didaktiky fyziky

Ing Peter Tatarko, PhD.

Názov semestr. predmetu: Príprava a vlastnosti pokročilej keramiky I.

Počet hodín za semester: 3

Názov katedry a vysokej školy: Fakulta chemickej a potravinárskej technológie STU, Ústav anorganickej chémie, technológie a materiálov

Príloha E - Medzinárodná mobilita organizácie

(A) Vyslanie vedeckých pracovníkov do zahraničia na základe dohôd:

Krajina	D r u h d o h o d y					
	MAD, KD, VTS		Medziústavná		Ostatné	
	Meno pracovníka	Počet dní	Meno pracovníka	Počet dní	Meno pracovníka	Počet dní
Belgicko	Adriana	10				
	Czímerová					
	Anna Prnová	14				
Čína	Michal	14				
	Korenko					
Poľsko	Valéria	10				
	Bizovská					
	Helena	10				
	Páľková					
Počet vyslaní spolu	5	58				

(B) Prijatie vedeckých pracovníkov zo zahraničia na základe dohôd:

Krajina	D r u h d o h o d y					
	MAD, KD, VTS		Medziústavná		Ostatné	
	Meno pracovníka	Počet dní	Meno pracovníka	Počet dní	Meno pracovníka	Počet dní
Česko	Jiří Hybler	7			Lenka Blahová	97
Poľsko	Małgorzata Zimowska	11				
Rakúsko					Christina Atzenhofer	4
Turecko					Nadide Fulden Onan	89
Veľká Británia					Amit Mahajan	4
Počet prijatí spolu	2	18			4	194

(C) Účast' pracovníkov pracoviska na konferenciách v zahraničí (nezahrnutých v "A"):

Krajina	Názov konferencie	Meno pracovníka	Počet dní
Belgicko	FPMC	Zoltán Lenčes	4
		Pavol Šajgalík	4
Česko	EUROCORR&ICC	Niketan Patel	7
	Ksappm	Anna Prnová	4

	MolS	Valéria Bizovská	3
		Jana Madejová	3
		Helena Páľková	3
	MQD	Anna Prnová	2
Čína	CICC-10	Pavol Šajgalík	4
Estónsko	Kfistr&Ifwa	Dušan Galusek	3
Francúzsko	MEDEA	Eva Scholtzová	5
Grécko	GraW	Ondrej Hanzel	6
	iPROMEDAI	Valéria Bizovská	5
		Peter Boháč	5
India	CORCON	Niketan Patel	6
	ICAGST	Peter Šimurka	6
	ICMS	Juraj Bujdák	11
	RAMET	Jozef Noga	8
Japonsko	ACA	Eva Scholtzová	7
	ISSNOX5	Zoltán Lenčes	6
	TDM	Oľga Malkin	10
		Vladimír Malkin	10
Maďarsko	ECERS	Roman Bystrický	6
		Dušan Galusek	5
		Ondrej Hanzel	6
		Zoltán Lenčes	6
		Pavol Šajgalík	6
		Peter Tatarko	6
	JTACC	Mária Chromčíková	4
		Anna Prnová	6
Nemecko	ICReHeChP	Stanislav Komorovský	5
Poľsko	CESTCh	Stanislav Kedžuch	4
		Jozef Noga	4
	CPCS&PSchSC	Zoltán Lenčes	3
	Teaming	Dušan Galusek	2
Portugalsko	PAWC	Juraj Bujdák	8
Rakúsko	MMQC	James Richard Asher	6
		Stanislav Komorovský	6
		Oľga Malkin	6
		Vladimír Malkin	6
Slovinsko	ICMT25	Martin Kontrík	5
		František Šimko	5
Španielsko	ICC	Valéria Bizovská	6
		Peter Boháč	6
		Juraj Bujdák	8
		Ľuboš Jankovič	6
		Peter Komadel	6
		Jana Madejová	6
		Helena Páľková	6
		Lukáš Petra	6
		Eva Scholtzová	5
	ICoC	Alexander Čeklovský	4
	ISCGL	Anna Prnová	8
	RfMM	Jozef Noga	3
Turecko	ICG	Dušan Galusek	4
	JSF	Miroslav Boča	3
USA	ICACC	Ondrej Hanzel	9
		Zoltán Lenčes	9
		Pavol Šajgalík	9

	ICS	Dušan Galusek	8
	MS&T17	Zoltán Lenčéš	6
	PACRIM	Dušan Galusek	14
		Zoltán Lenčéš	8
		Pavol Šajgalík	8
	SS	Jozef Noga	9
Spolu	37	65	384

Vysvetlivky: MAD - medziakademické dohody, KD - kultúrne dohody, VTS - vedecko-technická spolupráca v rámci vládnych dohôd

Skratky použité v tabuľke C:

ACA - 5th Annual Conference of Analytix

CESTCh - 15th Central European Symposium on Theoretical Chemistry

CICC-10 - International Conference on High-Performance Ceramics

CORCON - International Conference and Exhibition on Corrosion

CPCS&PSchSC - 11th Conference of the Polish Ceramic Society and Polish-Slovak-Chinese Seminar on Ceramics

ECERS - 15th Conference and Exhibition of the European Ceramic Society

ECERS - 15th Conference and Exhibition of the European Ceramics

EUROCORR&ICC - EUROCORR 2017 and 20th International Corrosion Congress

FPMC - Francis Cambier Symposium "Future Perspectives on the magical world of ceramics"

GraW - Graphene Week

ICACC - International Conference and Exposition on Advanced Ceramics

ICAGST - International Conference on Advances in Glass

ICC - 16th International Clay Conference

ICC - 16th International Clay Conference

ICG - ICG Annual Meeting and 32nd Siceam Glass Symposium

ICMS - 2th International Conference on Material Science

ICMT25 - 25th International Conference on Materials and Technology

ICoC - 7th International Colloids Conference

ICReHeChP - 12th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics

ICS - International Conference on Sintetic 2017

iPROMEDAI - Seminár: "iPROMEDAI Young Scientist Forum"

ISCGL - 12th International Symposium on Crystallization in Glasses and Liquids

ISSNOX5 - 9th International Symposium on Nitrides

JSF - 7th Joint Scientific forum between the SAS and TUBITAK

JTACC - 1st Journal of Thermal Analysis and Calorimetry Conference and 6th V4 (Joint

Czech-Hungarian-Polish-Slovakian) Thermoanalytical Conference

Kfiser&Ifwa - Workshope: "The key factors for impact strategic research and innovation funding in a view of widening actions"

Ksappm - 19. ročník Konference o speciálních anorganických pigmentech a práškových materiálech

MEDEA - Workshope 2017: "Medea softféru"

MMQC - Xth Workshop on Modern Methods in Quantum Chemistry

MolS - "Molekulová spektroskopie 2017"

MQD - Seminár: "Malvern/Quantachrome Dataphysics"

MS&T17 - Materials Science and Technology

PACRIM - The 12th Pacific Rim Conference on Ceramic and Glass Technology

PAWC - 16th International Photodynamic Association World Congress

RAMET - Recent Advances in Many-Electron Theory

RfMM - Sympóziu: "Routes of formation of medium-size molecules at low"

SS - 57th Sanibel Symposium

TDM - "Theoretical Design of Materials with Innovative Functions Based on Element Strategy and Relativistic Electronic Theory"

Teaming - Workshop on Teaming

Príloha F - Vedecko-popularizačná činnosť pracovníkov organizácie SAV

Meno	Spoluautori	Typ¹	Názov	Miesto zverejnenia	Dátum alebo počet za rok
Ing. Viliam Pavlík, PhD.		PB	Projekt Iniciatívy mladých vedcov: „Roadshow“ mladých vedcov po školách, 3 prednášky	Gymnázium J. Hollého v Trnave, Stredná odborná škola na Nerudovej ulici v Hlohovci, Gymnázium na Ul. 17.novembra v Topoľčanoch	3

¹ PB - prednáška/beseda, TL - tlač, TV - televízia, RO - rozhlas, IN - internet, EX - exkurzia, PU - publikácia, MM - multimédiá, DO - dokumentárny film