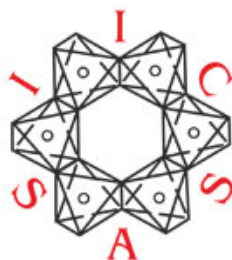


# Ústav anorganickej chémie SAV



## Správa o činnosti organizácie SAV za rok 2021

Bratislava  
január 2022

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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.

**Adresa:** Dúbravská cesta 9, 845 36 Bratislava 45

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

**Tel.:** 02/59410401

**E-mail:** uachsekr@savba.sk

**Názvy a adresy organizačných zložiek a detašovaných pracovísk:**

Organizačné zložky: nie sú

Detašované pracoviská:

- **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 organizačných zložiek a detašovaných pracovísk:**

Organizačné zložky: nie sú

Detašované pracoviská:

- **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.

**Členovia Snemu SAV za organizačné zložky:**

nie sú

**Typ organizácie:** Rozpočtová od roku 1953

## 1.2. Údaje o zamestnancoch

Tabuľka 1a Počet a štruktúra zamestnancov

Štruktúra zamestnancov	K	K		K do 35		F	P	T	O
		M	Ž	M	Ž				
<b>Celkový počet zamestnancov</b>	75	39	36	8	7	71	59.49	43.51	0
<b>Vedeckí pracovníci</b>	49	31	18	6	4	46	37.34	37.26	0
<b>Odborní pracovníci VŠ</b> (výskumní a vývojoví zamestnanci <sup>1</sup> )	7	5	2	2	0	6	6.86	5.83	0
<b>Odborní pracovníci VŠ</b> (ostatní zamestnanci <sup>2</sup> )	5	1	4	0	2	5	3.8	0.42	0
<b>Odborní pracovníci ÚS</b>	10	2	8	0	0	10	9.09	0	0
<b>Ostatní pracovníci</b>	4	0	4	0	1	4	2.4	0	0

<sup>1</sup> odmeňovaní podľa 553/2003 Z.z., príloha č. 5<sup>2</sup> odmeňovaní podľa 553/2003 Z.z., príloha č. 3 a č. 4

K – kmeňový stav zamestnancov v pracovnom pomere k 31.12.2021 (uvádzať zamestnancov v pracovnom pomere, vrátane riadnej materskej dovolenky, zamestnancov pôsobiach v zahraničí, v štátnych funkciách, členov Predsedníctva SAV, zamestnancov pôsobiach v zastupiteľských zboroch)

F – fyzický stav zamestnancov k 31.12.2021 (bez riadnej materskej dovolenky, zamestnancov pôsobiach v zahraničí v štátnych funkciách, členov Predsedníctva SAV, zamestnancov pôsobiach v zastupiteľských zboroch)

P – celoročný priemerný prepočítaný počet zamestnancov

T – celoročný priemerný prepočítaný počet riešiteľov projektov

O – celoročný priemerný prepočítaný počet obslužného personálu podieľajúceho sa na riešení projektov (technikov, laborantov, projektových manažérov a pod.) mimo zamestnancov v administratívne, správe a údržbe budov, upratovačiek, vodičov a pod.

M, Ž – muži, ženy

Tabuľka 1b Štruktúra vedeckých pracovníkov (kmeňový stav k 31.12.2021)

Rodová skladba	Pracovníci s hodnosťou				Vedeckí pracovníci v stupňoch		
	DrSc.	CSc./PhD.	prof.	doc.	I.	II.a.	II.b.
<b>Muži</b>	6	27	4	5	6	14	11
<b>Ženy</b>	2	16	0	2	2	8	8

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

Veková štruktúra	< 31		31-35		36-40		41-45		46-50		51-55		56-60		61-65		> 65	
	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
<b>Muži</b>	2	2.0	7	5.7	5	5.0	2	2.0	8	7.2	1	0.6	2	1.5	1	1.0	5	2.5
<b>Ženy</b>	2	2.0	2	1.4	1	0.8	3	3.2	4	4.0	2	1.6	1	1.0	2	2.0	0	0.0

A - Prepočet bez zohľadnenia úväzkov zamestnancov

B - Prepočet so zohľadnením úväzkov zamestnancov

Tabuľka 1d Priemerný vek zamestnancov organizácie k 31.12.2021

	Kmeňoví zamestnanci	Vedeckí pracovníci	Riešitelia projektov
<b>Muži</b>	45.8	45.4	45.7
<b>Ženy</b>	46.6	44.4	45.8
<b>Spolu</b>	46.2	45.0	45.7

**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 2021 nezaznamenal žiadne zásadné zmeny v organizačnej štruktúre. Udialo sa iba niekoľko drobných personálnych zmien súvisiacich s prirodzenou obmenou z dôvodu odchodu do dôchodku.

Prepočítaný počet pracovníkov v roku 2021 je na úrovni 59,49 FTE, čo je mierne vyšší stav v porovnaní s rokom 2020 (57,46). V roku 2021 bol priemerný vek všetkých pracovníkov ústavu 46,2 roka a priemerný vek vedeckých pracovníkov 45,0. Vzhľadom na to, že nedochádza k plynulej generáčnej výmene, postupne sa zvyšuje aj priemerný vek zamestnancov. V roku 2021 sa na ústave zamestnali traja mladí vedeckí pracovníci, dvaja boli PhD študenti školení na ÚACH SAV, ktorí úspešne obhájili svoju prácu a jedna zamestnankyňa je zo zahraničia. V priebehu roka ukončili zamestnanecký pomer štyria zamestnanci, z toho dve zamestnankyne z dôvodu dosiahnutia dôchodkového veku. Zamestnávanie mladých schopných post-doktorandov na ústave je naďalej jednou z hlavných priorít, avšak nevieme ju v požadovanej miere naplniť. 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.

## 2. Vedecká činnosť

### 2.1. Domáce projekty

Tabuľka 2a Domáce projekty riešené v roku 2021

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	10	3	108015	108015	-	-	-	9073
2. Projekty APVV	6	6	-	-	308760	246879	-	83617
3. Projekty EŠIF/OP ŠF	0	2	-	-	-	-	-	145830
4. Projekty SASPRO, MoRePro	0	0	-	-	-	-	-	-
5. Iné projekty (FM EHP, Vedecko-technické projekty, na objednávku rezortov a pod.)	1	0	2000	2000	-	-	-	-

A - organizácia je nositeľom projektu

B - organizácia sa zmluvne podieľa na riešení projektu

Tabuľka 2b Domáce projekty podané v roku 2021

Štruktúra projektov	Miesto podania	Organizácia je nositeľom projektu	Organizácia sa zmluvne podieľa na riešení projektu
1. Účasť na nových výzvach APVV r. 2021	-	6	3
2. Projekty výziev EŠIF podané r. 2021	Bratislava		
	Regióny		

#### Projekty podané v rámci všeobecnej výzvy 2021

**Názov projektu:** Fluoridové systémy pre zelenú metalurgiu a elektrochémiu bez tvorby CO<sub>2</sub>

**Evidenčné číslo projektu:** APVV-21-0368

**Acronym:** FRONTAL

**Podávateľ projektu:** Ústav anorganickej chémie SAV

**Partner/i:** Fyzikálny ústav, SAV

**Stav:** podaný

**Názov projektu:** Vývoj nových keramických materiálov komplexného zloženia pre extrémne aplikácie

**Evidenčné číslo projektu:** APVV-21-0402

**Acronym:** ComCer

**Podávateľ projektu:** Ústav anorganickej chémie SAV

**Partner/i:** Ústav materiálového výskumu SAV

**Stav:** podaný

**Názov projektu:** Horčík ako čisté obnoviteľné palivo

**Evidenčné číslo projektu:** APVV-21-0501

**Acronym:** MagFuel

**Podávateľ projektu:** Ústav materiálov a mechaniky strojov SAV

**Partner/i:** Ústav anorganickej chémie SAV

**Stav:** podaný

**Názov projektu:** Aditívna výroba pokročilej poréznej sklo-keramickej membrány na čistenie odpadovej vody

**Evidenčné číslo projektu:** APVV-21-0235

**Acronym:** 3DClearStream

**Podávateľ projektu:** Trenčianska univerzita Alexandra Dubčeka v Trenčíne

**Partner/i:** Ústav anorganickej chémie SAV

**Stav:** podaný

**Názov projektu:** Smerom k nanotechnológiám využívajúcim bioaktívne častice/molekuly v boji proti mikrobiálnym biofilmom.

**Evidenčné číslo projektu:** APVV-21-0302

**Akronym:** NIPOFABs

**Podávateľ projektu:** Prírodovedecká fakulta UK Bratislave,

**Partner/i:** Ústav anorganickej chémie SAV

**Stav:** podaný

### **Bilaterálne projekty**

**Názov projektu:** Vysokoteplotná Ramanova spektroskopia tavenín a skiel

**Evidenčné číslo projektu:** SK-RU-RD-21-0016

**Acronym:** HITERMEG

**Podávateľ projektu:** Ústav anorganickej chémie SAV

**Partner/i:** TnAD

**Stav:** podaný

**Názov projektu:** Vývoj nových metód spájania vysoko-entropických keramických materiálov

**Evidenčné číslo projektu:** APVV-SK-CZ-RD-21-0089

**Acronym:** JoinHEC

**Podávateľ projektu:** Ústav anorganickej chémie SAV

**Partner/i:** Ústav fyziky materiálu AVČR Brno, Česká republika

**Stav:** podaný

**Názov projektu:** Rozpustnosť oxidov a plynov v roztavenom systéme  $KF-AlF_3$

**Evidenčné číslo projektu:** SK-CN-21-0016

**Acronym:** SOXIGA

**Podávateľ projektu:** Ústav anorganickej chémie SAV

**Partner/i:** Northeastern University, Shenyang, Čína

**Stav:** nepodporený

**Názov projektu:** Vysokoteplotné karbidy pre aplikácie v extrémnych podmienkach

**Evidenčné číslo projektu, výzva:** APVV-SK-SRB-0022

**Acronym:** CerEx

**Podávateľ projektu:** Ústav anorganickej chémie SAV

**Partner/i:** Belgrade University, Institute for Nuclear Sciences, Belgrade, Srbsko

**Stav:** schválený

## 2.2. Medzinárodné projekty

## 2.2.1. Medzinárodné projekty riešené v roku 2021

Tabuľka 2c Medzinárodné projekty riešené v roku 2021

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		
<b>1. Projekty Horizont 2020 a Horizont Európa</b>	0	1	-	-	-	-	4018	28401
<b>2. Projekty ERA.NET, ESA, JRP</b>	2	0	49996	49996	-	-	-	-
<b>3. Projekty COST</b>	0	0	-	-	-	-	-	-
<b>4. Projekty EUREKA, NATO, UNESCO, CERN, IAEA, IVF, ERDF a iné</b>	0	1	-	-	-	-	4167	-
<b>5. Projekty v rámci medzivládnych dohôd</b>	0	0	-	-	-	-	-	-
<b>6. Bilaterálne projekty MAD, Mobility, Open Mobility</b>	2	0	1351	1000	-	-	-	-
<b>7. Bilaterálne projekty ostatné</b>	2	1	-	-	-	-	-	-
<b>8. Podpora MVTS z národných zdrojov okrem SAV (APVV a iné)</b>	1	0	-	-	1823	1823	-	-
<b>9. SAS-UPJŠ ERC Visiting Fellowship Grants</b>	0	0	-	-	-	-	-	-
<b>10. Iné projekty</b>	0	0	-	-	-	-	-	-

A - organizácia je nositeľom projektu

B - organizácia sa zmluvne podieľa na riešení projektu



### 2.2.2. Medzinárodné projekty Horizont Európa podané v roku 2021

Tabuľka 2d Počet projektov Horizont Európa v roku 2021

	A	B
<b>Počet podaných projektov Horizont Európa</b>		

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 Európskych štrukturálnych a investičných fondov v ďalších výzvach

## 2.3. Výber najvýznamnejších výsledkov vedeckej práce organizácie v roku 2021

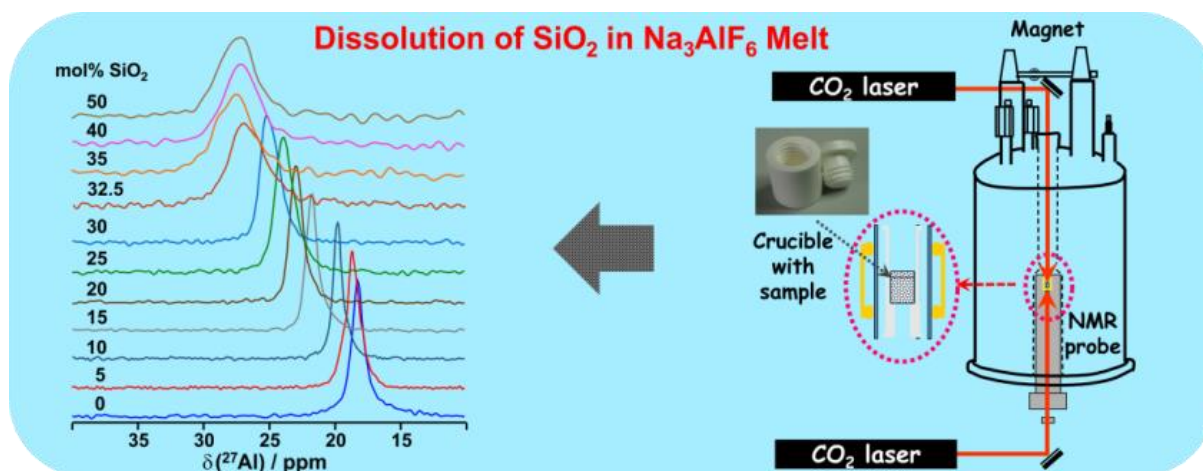
### 2.3.1. Výsledky na báze základného výskumu

#### VZŤAH MEDZI ŠTRUKTÚROU A FYZIKÁLNO-CHEMICKÝMI VLASTNOSTAMI TAVENINOVÉHO ELEKTROLYTU NA BÁZE $\text{Na}_3\text{AlF}_6\text{-SiO}_2$ PRE ELEKTROLYTICKÚ VÝROBU SOLAR GRADE KREMÍKA (SoG-Si)

František ŠIMKO, Michal KORENKO

Elektrolýza z roztavenej soli je nový spôsob výroby kremíka pre solárne fotovoltaické aplikácie (SoG-Si), ktorý umožňuje zníženie ekonomických nákladov, spotreby energie a jeho prípadnú recykláciu. Pochopenie vzťahov medzi štruktúrou roztaveného elektrolytu a jeho fyzikálno-chemickými vlastnosťami je nevyhnutné pre optimalizáciu parametrov elektrolýzy, no potrebné informácie sú v tejto oblasti stále veľmi obmedzené. Predchádzajúci skrining roztavených elektrolytov poukázal na to, že s ohľadom na kvalitu kremíkoveho depozitu a efektívnosť procesu sú taveniny na báze  $\text{Na}_3\text{AlF}_6$  veľmi sľubným médium pre jeho elektrolýtickú výrobu.

Výsledkom štúdie bola kompletná štruktúrna vysokoteplotná NMR charakterizácia roztaveného systému na báze  $\text{Na}_3\text{AlF}_6\text{-SiO}_2$ , charakterizácia jeho elektrolaktívnych iónových častíc ako aj určenie štruktúry jeho ďalších štruktúrnych častíc. Veľmi dôležitým zistením bolo určenie vplyvu prítomnosti polymerizovaných častíc na zvýšenie viskozity a elektrickej vodivosti elektrolytu.



Obr. 1. Vysokoteploté NMR spektrá izotopu  $^{27}\text{Al}$  roztaveného elektrolytu (pri  $1025^\circ\text{C}$ ) s rôznym prídavkom  $\text{SiO}_2$  a schématické znázornenie meracieho zariadenia.

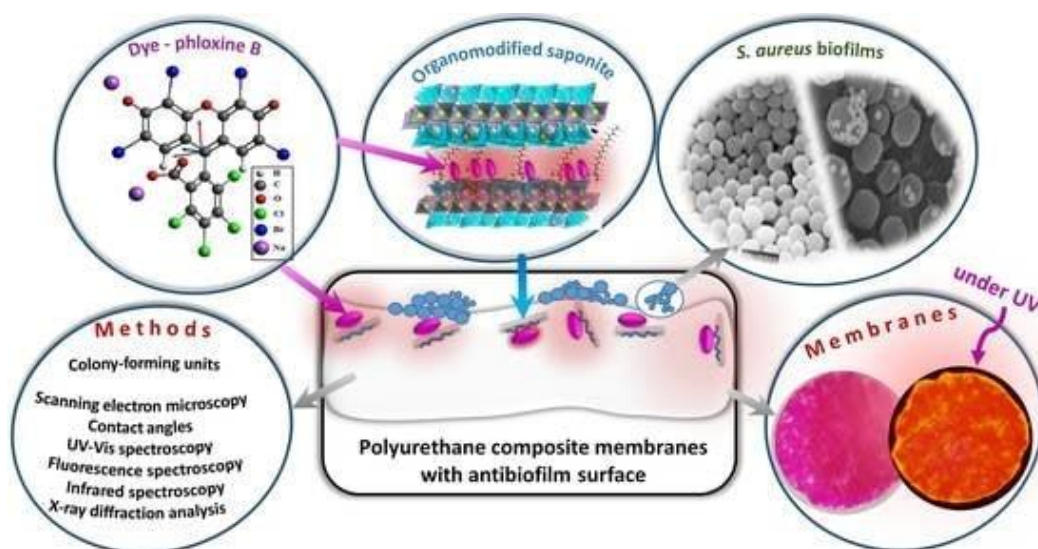
#### Publikácia:

ŠIMKO František\*, RAKHMATULLIN Aydar, KORENKO Michal, BESSADA Catherine. Structural Correlations and Chemistry of the  $\text{Na}_3\text{AlF}_6\text{-SiO}_2$  Melt as an Electrolyte for the Solar Grade Silicon (SOG-Si) Electrowinning. In Journal of Molecular Liquids, 2021, Vol. 328, p. 115453; Doi: 10.1016/j.molliq.2021.115453 (IF: 6.165; Q1)

## OPTIMALIZÁCIA PRÍPRAVY NANOMATERIÁLOV NA BÁZE VRSTEVNATÝCH HLINITOKREMIČITANOV A ORGANICKÝCH FARBÍV

Martin BARLOG, Peter BOHÁČ, Juraj BUJDÁK, PÁLKOVÁ Helena, Tímea ŠIMONOVÁ

Dôležitou skupinou materiálov na báze vrstevnatých kremičitanov sú hybridné anorganicko-organické materiály, v ktorých funkčnou zložkou sú rôzne organické farbivá. Medzi zložkami prebiehajú rôzne interakcie a javy, čo si vyžiadalo rozsiahly výskum a hĺbkovú analýzu experimentálnych dát. Podarilo sa odhaliť mechanizmy interakcií organických farbív s vrstevnatými kremičitanmi, čo pomohlo ozrejmiť výskyt niektorých javov, ako sú napr. tvorba molekulových agregátov a pokles fotoaktivity [1]. Vypracovali sa rôzne stratégie pre prípravu hybridných tuhých látok, aby sa v čo najväčšej miere zachovala fotoaktivita farbív. Jedným z dôležitých krokov je modifikácia povrchu nanočastíc silikátu pomocou organických surfaktantov [2-3]. Okrem vplyvu na aktivitu farbív, je tento typ modifikácie nevyhnutný pri príprave nanokompozitov, aby sa dosiahla kompatibilita nanočastíc s polymermi [4]. Optimalizáciou parametrov syntéz sa podarilo pripraviť kompozity polymérov s významnými antimikrobiálnymi vlastnosťami, v ktorých ako významná antimikrobiálna zložka vystupoval fotosenzibilizátor floxín B (Obr).



*Schematické znázornenie prípravy povrchov polymérov modifikovaných s nanočasticami organosaponit-farbivo.*

### Publikácie

1. ŠIMONOVÁ, T.\*\* - MÉSZÁROS, R. - SEBECHLEBSKÁ, T. - BUJDÁK, J.\*\* Non-Arrhenius kinetics and slowed-diffusion mechanism of molecular aggregation of a rhodamine dye on colloidal particles. In Physical Chemistry Chemical Physics, 2021, vol. 23, no. 32, p. 17177-17185. (2020: 3.676 - IF, Q1 - JCR, 1.053 - SJR, Q1 - SJR). ISSN 1463-9076.
2. BOHÁČ, P.\*\* - SASAI, R. - SOONTORNCHAIYAKUL, W. - CZÍMEROVÁ, A. - BUJDÁK, J. Resonance energy transfer between cyanine dyes in hybrid films of layered silicate prepared by layer-by-layer method. In Applied Clay Science, 2021, vol. 202, p. 105985-1-105985-9. (2020: 5.467 - IF, Q1)
3. BARLOG, M.\*\* - PÁLKOVÁ, H. - BUJDÁK, J. Luminescence of a laser dye in organically-modified layered silicate pigments. In Dyes and Pigments, 2021, vol. 191, p. 109380-1-109380-11. (2020: 4.889 - IF, Q1).
4. DADI, N. C. T. - BUJDÁK, J.\*\* - MEDVECKÁ, V. - PÁLKOVÁ, H. - BARLOG, M. - BUJDÁKOVÁ, H.\*\* Surface characterization and anti-biofilm effectiveness of hybrid films of polyurethane functionalized with saponite and phloxine B. In Materials, 2021, vol. 14, p. 7583-1-7583-21. (3.623 - IF, Q1).

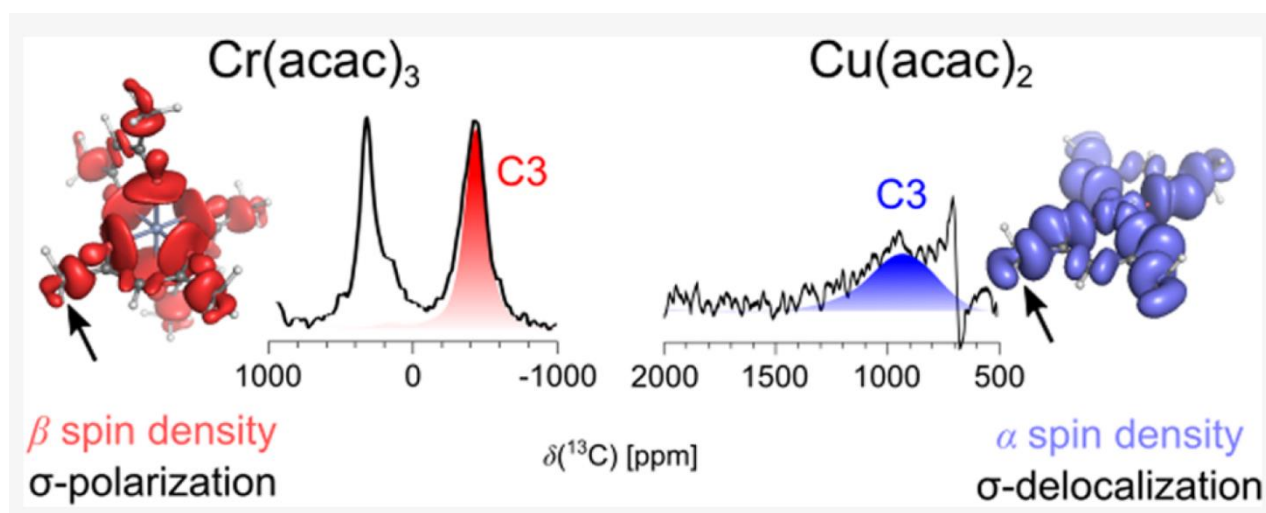
### Projekt

APVV-18-0075 Povrchy polymérov modifikované vrstevnatými nanočasticami a fotoaktívnymi farbivami

## HLBŠIE POROZUMENIE NMR SPEKTRÁM PARAMAGNETICKÝCH KOMPLEXOV PRECHODNÝCH KOVOV

Jan NOVOTNÝ, Stanislav KOMOROVSKÝ

Nukleárna magnetická rezonancia (NMR) je výnimočná technika, ktorá má široké uplatnenie vo vede, medicíne a priemysle. NMR spektroskopia sa napríklad používa na charakterizáciu nových protirakovinových liekov alebo na štúdium spracovania jadrového odpadu. NMR spektrá obsahujú množstvo užitočnej informácie o elektrónovej štruktúre paramagnetických látok. Na rozdiel od NMR spektroskopie diamagnetických látok, je NMR paramagnetických molekúl relatívne nepreskúmaná a náročná vedecká oblasť. Táto práca obsahuje podrobnú experimentálnu a teoretickú štúdiu dvoch paramagnetických zlúčenín v tuhom stave [Cr(III)] a [Cu(II)] s výrazne odlišnou elektrónovou štruktúrou. Vôbec prvýkrát boli pozorované a analyzované extrémne odtienené  $^{13}\text{C}$  NMR posuny, 900-1200 ppm. Merané signály sú vysvetlené na základe elektrónovej a spinovej štruktúry a dvoch spinových delokalizačných mechanizmov, konjugácie v  $\pi$ -priestore a hyperkonjugácie v  $\sigma$ -priestore. Tento príspevok poskytuje návod pre budúce skúmanie NMR signálov komplexných paramagnetických systémov.



### Publikácia:

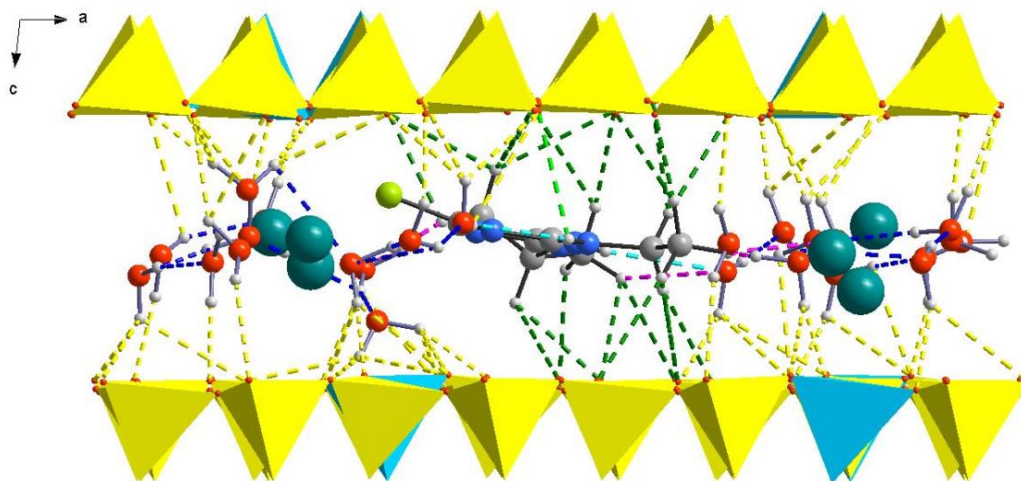
NOVOTNÝ, Jan\* – JEREMIAS, Lukáš\* – NIMAX, Patrick – KOMOROVSKÝ, Stanislav – HEINMAA, Ivo – MAREK, Radek\*\*. Crystal and substituent effects on paramagnetic NMR shifts in transition-metal complexes. In *Inorganic Chemistry*, 2021, vol. 60, no. 13, p. 9368-9377. (2020: 5.165 – IF, Q1 – JCR)

## ŠTÚDIUM VPLYVU MODIFIKÁCIE SMEKTITOV NA STABILITU ICH INTERKALÁTOV S HERBICÍDOM ATRAZÍNOM *AB INITIO* DFT METÓDOU

Daniel MORENO RODRÍGUEZ, Ľuboš JANKOVIČ, Eva SCHOLTZOVÁ

V práci bola teoreticky študovaná stabilita štruktúr s interkalovaným herbicídnom atrazínom v ílových mineráloch na báze smektitov, v beidellite (Bd) a montmorillonite (Mt) *ab initio* DFT metódou. V štúdiu boli použité modely interkalovaného atrazínu v čistých smektitoch ako aj v modifikovaných organickým surfaktantom, tetrametylfosfóniovým kationom. Analyzované vodíkové väzby a interkalačná energia ( $E_{\text{int}}$ ) reprezentujúca mieru stability jednotlivých organoílov ukázali, že jednoznačne stabilnejšie sú štruktúry na báze Bd, ktorý sa vyznačuje substitúciami v tetraédrických sieťach ( $\text{Al}^{3+}/\text{Si}^{4+}$ ) a modifikácia smektitu organickým kationom (TMP) výrazne prispieva k zvýšeniu stability štruktúry herbicíd-smektit pre obidva smektity. ( $E_{\text{int}}$  - Bd: -67.6; -221.1; kJ/mol a Mt: -48.1; -189.0 kJ/mol).





Vodíkové väzby v A-Bd modeli ako príklad: zelená ( $C-H \cdots O_b$ ), cyklaménová ( $C-H \cdots O_w$ ), žltá ( $O_w-H \cdots O_b$ ), modrá ( $O_w-H \cdots O_w$ ), tyrkysová ( $N-H \cdots O_w$ ), červená ( $N-H \cdots O_b$ ); b-pohľad.

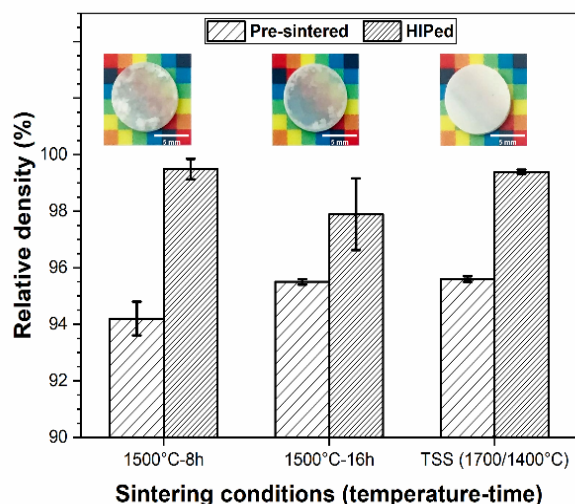
#### Publikácia:

MORENO RODRÍGUEZ, Daniel\*\* - JANKOVIČ, Ľuboš - SCHOLTZOVÁ, Eva - TUNEGA, Daniel. Stability of atrazine-smectite intercalates: Density functional theory and experimental study. In MINERALS-BASEL, 2021, vol. 11, no. 6, p. 554-1-554-20. (2020: 2.644 - IF, Q2 – JCR) Typ: ADCA

### TRANSLUCENTNÁ $Y_2O_3$ KERAMIKA PRIPRAVENÁ VYROBENÁ Z KOMERČNÉHO NANOPRÁŠKU TVAROVANÉHO ZA SUCHA

Aliasghar NAJAFZADEHKHOEE, Jaroslav SEDLÁČEK, Dušan GALUSEK

Výroba vysoko kompaktných surových/nespečených telies je kľúčovou stratégiou na dosiahnutie vysokej hustoty a transparentnosti polykrystalickej keramiky vyrobenej práškovou metalurgiou. Tento prístup však komplikuje proces tvarovania. Hoci vysoká spekateľnosť nanokeramických práškov otvorila sľubnú cestu k dosiahnutiu vysokohutných homogénnych telies, takýto potenciál nebol nikdy využitý na zjednodušenie výroby transparentnej keramiky. Práca skúma, či použitie nano- $Y_2O_3$  prášku umožní výrobu transparentnej  $Y_2O_3$  keramiky z nespečených vzoriek s nízkou počiatočnou hustotou. Komerčný nano  $Y_2O_3$  prášok s veľkosťou častíc približne 30 nm bol tvarovaný jednoosovým lisovaním, zhutnený predspekáním pri teplote 1500 °C s následným žiarovým izostatickým lisovaním. Vďaka vynikajúcej spekateľnosti nanoprášku  $Y_2O_3$  prášku bolo možné aj napriek nízkej počiatočnej hustote získať vysokohutné priesvitné  $Y_2O_3$  vzorky.



Obr. Relatívna hustota vzoriek vyrobených žiarovým izostatickým lisovaním pred a po HIP-e a optické fotografie HIP-ovaných vzoriek (hrúbka 1 mm) umiestnených priamo na pozadí.

#### Publikácia

NAJAFZADEHKHOEE, Aliasghar - TALIMIAN, Ali - SEDLÁČEK, Jaroslav - LISNICHUK, M - HVIZDOŠ Pavol – GALUSEK Dušan Translucent yttrium oxide ceramics from low-density green bodies shaped by uniaxial pressing, Journal of the European Ceramic Society, 2021, under review.

## SKÚMANIE KORODOVANÉHO POVRCHU HISTORICKÝCH SKIEL MIKRO-RAMANOVOU SPEKTROSKOPIOU.

Mária CHROMČÍKOVÁ, Marek LIŠKA

Korodovaný povrch historických skiel sa skúmal mikro-Ramanovou spektroskopiou. Súborné spektrá získané laterálnym a stratifikovaným mapovaním sa analyzovali metódou PCA (Principal Components Analysis), ktorá poskytla počet lineárne nezávislých spektier v skúmanom súbore. Následne sa metódou MCR (Multivariate Component Analysis) získali Ramanove spektrá nekorodovaného skla a jednotlivých korózných produktov (tzv. loadings) a ich relatívne zastúpenie (tzv. scores) v jednotlivých meraných bodoch. Správnosť získaných výsledkov sa potvrdila porovnaním výsledkov získaných laterálnym a stratifikovaným mapovaním. Na základe dominantných scores sa zobrazila laterálna distribúcia jednotlivých korózných produktov.

HG3OX										HG6OX										HG8OX									
1	1	2	2	2	2	2	2	2	2	1	1	1	1	1	1	3	1	1	1	1	1	2	2	2	2	2	2	2	2
1	2	2	2	2	2	2	2	2	1	3	1	2	1	1	1	3	3	1	1	1	1	2	2	2	2	2	2	1	3
3	2	2	2	2	2	2	2	2	3	3	1	1	1	1	1	1	1	3	1	1	1	2	2	2	2	2	2	3	3
2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
1	2	1	2	1	1	1	1	1	1	2	1	1	1	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
1	2	1	1	1	1	1	2	1	1	1	1	1	1	1	1	3	1	1	1	1	1	2	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	2	2	1	1	1	1	1	1	1	1	1	1	1	2	2	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	2	2	1	1	1	1	1	1	1	1	1	1	1	2	2	1	1	1	1	1	1
1	1	1	1	2	1	1	1	2	1	1	1	1	1	1	1	3	1	1	1	1	1	2	1	1	1	1	1	1	1
1	1	2	2	1	2	1	1	1	2	1	1	1	1	1	1	1	1	1	1	1	1	2	2	1	2	1	1	1	2

Distribúcia korózných produktov na povrchu vzoriek HG3OX, HG6OX, a HG8OX (1 - natívne sklo, 2, 3 – korózne produkty)

### Publikácia

HRUŠKA B – NOWICKA A – CHROMČÍKOVÁ M – GREINER-WRONA E – SMOLÍK J – SOLTÉZS V – LIŠKA M Raman spectroscopic study of corroded historical glass. In International Journal of Applied Glass Science, 2021, vol. 12, no. 4, p. 613-620. (IF 2.029, Q2)

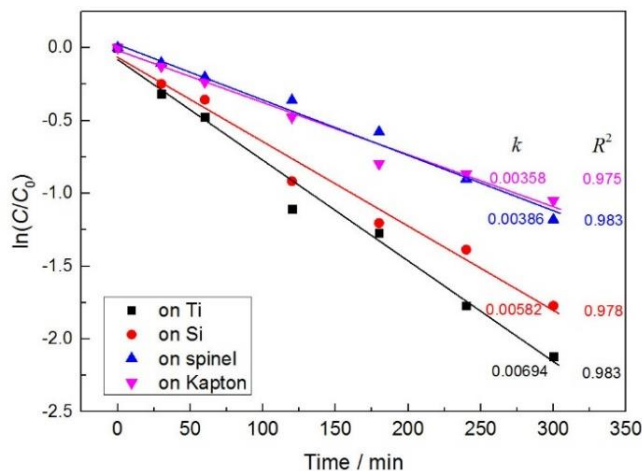
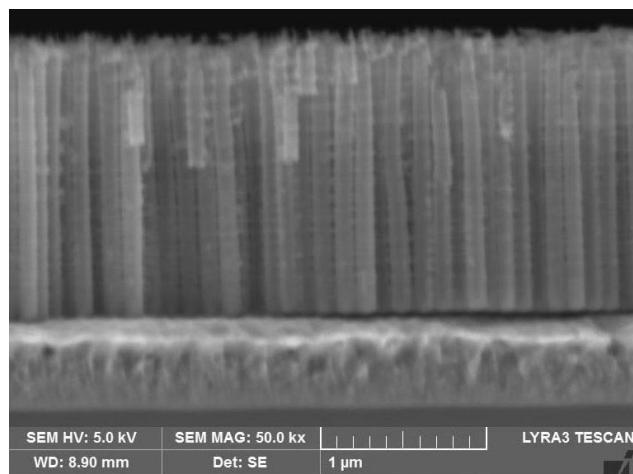
### 2.3.2. Výsledky aplikačného typu

## PRÍPRAVA A FOTOKATALYTICKÁ AKTIVITA TiO<sub>2</sub> NANORÚROK SYNTETIZOVANÝCH NA TRANSPARENTNOM SPINELOVOM SUBSTRÁTE

Patrícia PETRISKOVÁ, Zoltán LENČEŠ

Za posledné dve dekády sa čoraz väčšia pozornosť kladie na čistenie odpadových vôd pomocou fotokatalyzátora TiO<sub>2</sub>. Z toho dôvodu bol výskum zameraný na prípravu TiO<sub>2</sub> nanorúrok (TNTs) na transparentnom keramickom materiáli (spinel - MgAl<sub>2</sub>O<sub>4</sub>) pomocou anodickej oxidácie Ti vrstvy nanosennej magnetronovou depozíciou. Vlastnosti TNTs boli porovnané s nanorúrkami pripravenými na troch iných substrátoch: monokryštalický Si substrát, polymérna fólia Kapton a kovová Ti fólia. Pomocou fotokatalytickej degradácie dvoch modelových polutantov rodamínu B (RhB) a bispfenolu A (BPA) sme dokázali, že v závislosti na použítom substráte účinnosť fotokatalytickej degradácie TNTs rastie od Kapton < spinel < Si < Ti. Nanorúrky vypěstované na Ti fólii majú najlepšiu fotokatalytickú aktivitu dosahujúcu 88% degradácie RhB a 36% degradácie BPA. Kinetický model pre degradáciu RhB najlepšie popisuje reakcia pseudo-prvého stupňa, zatiaľ čo degradáciu BPA lepšie popisuje reakcia fraktálneho pseudo-prvého stupňa. Výsledky výpočtu zvyškového napätia a deformácie na rozhraní substrát-TNTs ukázali, že materiál spinel-TNTs vykazuje najnižšie hodnoty napätia a deformácie, majú stabilnú štruktúru a dochádza iba k minimálnemu odlupovaniu

TNTs.



#### Publikácia:

PETRISKOVÁ, Patrícia – MONFORT, Olivier – SATRAPINSKY, Leonid – DOBROČKA, Edmund – PLECENIK, Tomáš – PLESCH, Gustav – PAPŠIK, Roman – BERMEJO, Raúl – LENČEŠ, Zoltán: Preparation and photocatalytic properties of TiO<sub>2</sub> nanotube arrays prepared on transparent spinel. *Ceramics International*, 47 (2021) 12970-12980. (4,527 – IF2020)

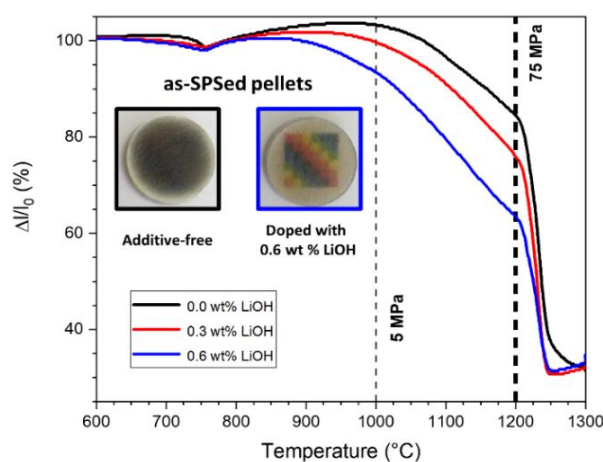
### 2.3.3. Výsledky na báze medzinárodnej spolupráce

#### POKROK PRI PRÍPRAVE TRANSPARENTNÉHO HOREČNATO-HLINITÉHO SPINELU – SPEKANIE PRI NÍZKYCH TEPLOTÁCH

Monika MICHÁLKOVÁ, Dušan GALUSEK

Cieľom tejto práce bolo odhaliť úlohu opticky neaktívnych defektov pri príprave transparentného horečnato-hlinitého spinelu a tieto poznatky následne zužitkovať pri vyvíjaní nových metód prípravy alebo zavedení nových spekacích prísad čo by umožnilo spekanie pri nižších teplotách. Vykonané štúdie ukázali, že:

1. spekanie MgAl<sub>2</sub>O<sub>4</sub> pomocou SPS pri nízkych teplotách znižuje kontamináciu vzoriek uhlíkom a umožňuje výrobu transparentného polykrystalického spinelu pri teplote nižšej ako 1300 °C,
2. štrukturálne defekty, ako je inverzia pri spinely, znižujú aktivačnú energiu spekania z cca. 800 kJ mol<sup>-1</sup> na 530 kJ mol<sup>-1</sup>,
3. prídavok LiOH ako spekacej prísady podporuje spekanie MgAl<sub>2</sub>O<sub>4</sub>, čo sa vysvetľuje koncentráciou kyslíkových vakancií a štrukturálnou inverziou,
4. LiOH je alternatívou ku konvenčným spekacím prísadám používaným na výrobu transparentného spinelu a
5. prídavok fluoridov prechodných kovov môže pomôcť zhutneniu a zároveň zaviesť opticky aktívny prvok do štruktúry MgAl<sub>2</sub>O<sub>4</sub>.



Krivky zhutnenia nedopovaných a  $\text{Li}^+$  dopovaných  $\text{MgAl}_2\text{O}_4$  vzoriek v závislosti od teploty spekania v SPS pri rýchlosti ohrevu  $100^\circ\text{C min}^{-1}$ .

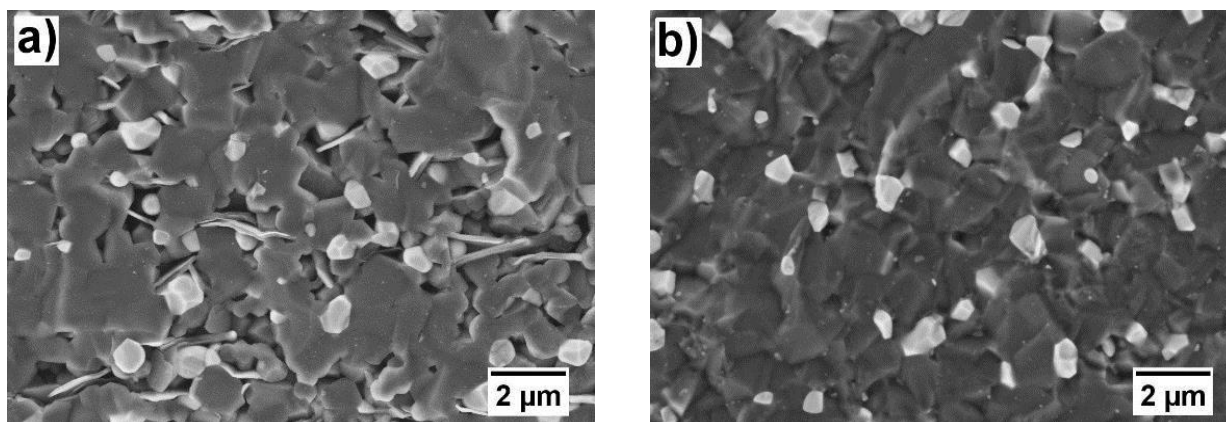
Publikácie:

[1] A. Talimian, V. Pouchly, H.F. El-Maghraby, K. Maca, D. Galusek, Impact of high energy ball milling on densification behaviour of magnesium aluminate spinel evaluated by master sintering curve and constant rate of heating approach, *Ceramics International*. 45 (2019) 23467–23474. <https://doi.org/10.1016/j.ceramint.2019.08.051>.

## ŠTÚDIUM VPLYVU ELEKTRICKÉHO POĽA NA IN-SITU TVORBU GRAFÉNOVÝCH PLATNIČIEK PRI REAKČNOM SPEKANÍ MATERIÁLOV NA BÁZE $\text{B}_4\text{C}$ - $\text{TiB}_2$

Hakan ÜNSAL, Ondrej HANZEL, Monika TATARKOVÁ, Peter TATARKO

Cieľom tejto práce bola príprava kompozitov  $\text{B}_4\text{C}$  s prídavkom 10 obj.%  $\text{TiB}_2$  pomocou reakčného spekania v elektrickom poli, kde sú finálne materiály tvorené in-situ reakciou medzi  $\text{B}_4\text{C}$ ,  $\text{TiO}_2$  a uhlíkovými sadzami. Bol jednoznačne preukázaný kombinovaný vplyv elektrického poľa a in-situ reakcií za vzniku veľkého množstva CO plynu na tvorbu elektrického oblúka. V dôsledku toho dochádzalo k výraznému lokálnemu prehriatiu na rozhraní  $\text{TiB}_2/\text{B}_4\text{C}$ , čo viedlo k čiastočnej dekompozícii zŕn  $\text{B}_4\text{C}$  za vzniku grafénových platničiek. Ak jeden z týchto dvoch faktorov nebol zapojený do procesu prípravy, napríklad pri žiarovom lisovaní bez elektrického poľa, resp. pri konvenčnom (bezreakčnom) spekaní práškov  $\text{B}_4\text{C}$  a  $\text{TiB}_2$  v elektrickom poli, nedochádzalo k tvorbe grafénových platničiek. Práca tiež navrhla inovatívny spôsob prevencie tejto dekompozície zŕn  $\text{B}_4\text{C}$ , využitím tzv. izolovaného reakčného spekania v elektrickom poli.



Obr. REM snímok lomového povrchu kompozitu  $\text{B}_4\text{C}$  - 10 vol.%  $\text{TiB}_2$  spekaného pri  $1800^\circ\text{C}$  pomocou: a) reakčného spekania v elektrickom poli, and b) izolovaného reakčného spekania v elektrickom poli.

Publikácia

ÜNSAL, Hakan - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - TATARKOVÁ, Monika -

DLOUHÝ, Ivo - TATARKO, Peter\*\*. In-situ graphene platelets formation and its suppression during reactive spark plasma sintering of boron carbide/titanium diboride composites. In Journal of the European Ceramic Society, 2021, vol. 41, no. 13, p. 6281-6289. (2020: 5.302 - IF, Q1 – JCR)



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

Tabuľka 2e Štatistika vybraných kategórií publikácií

<b>PUBLIKAČNÁ A EDIČNÁ ČINNOSŤ</b>	<b>Počet v r. 2021/ doplnky z r. 2020</b>
<b>1. Vedecké monografie a monografické štúdie vydané v domácich vydavateľstvách (AAB, ABB)</b>	<b>0 / 0</b>
<b>2. Vedecké monografie a monografické štúdie vydané v zahraničných vydavateľstvách (AAA, ABA)</b>	<b>0 / 0</b>
<b>3. Odborné monografie, vysokoškolské učebnice a učebné texty vydané v domácich vydavateľstvách (BAB, ACB, CAB)</b>	<b>0 / 0</b>
<b>4. Odborné monografie a vysokoškolské učebnice a učebné texty vydané v zahraničných vydavateľstvách (BAA, ACA, CAA)</b>	<b>0 / 0</b>
<b>5. Kapitoly vo vedeckých monografiách vydaných v domácich vydavateľstvách (ABD)</b>	<b>0 / 0</b>
<b>6. Kapitoly vo vedeckých monografiách vydaných v zahraničných vydavateľstvách (ABC)</b>	<b>2 / 0</b>
<b>7. Kapitoly v odborných monografiách, vysokoškolských učebniciach a učebných textoch vydaných v domácich vydavateľstvách (BBB, ACD)</b>	<b>0 / 0</b>
<b>8. Kapitoly v odborných monografiách, vysokoškolských učebniciach a učebných textoch vydaných v zahraničných vydavateľstvách (BBA, ACC)</b>	<b>0 / 0</b>
<b>9. Vedecké práce registrované v Current Contents Connect (ADCA, ADCB, ADDA, ADDB)</b>	<b>80 / 0</b>
<b>10. Vedecké práce registrované vo Web of Science Core Collection alebo Scopus (ADMA, ADMB, ADNA, ADNB)</b>	<b>5 / 1</b>
<b>11. Vedecké práce v ostatných domácich časopisoch (ADFA, ADFB)</b>	<b>0 / 0</b>
<b>12. Vedecké práce v ostatných zahraničných časopisoch (ADEA, ADEB)</b>	<b>0 / 0</b>
<b>13. Vedecké práce v domácich recenzovaných zborníkoch (AEDA)</b>	<b>0 / 0</b>
<b>14. Vedecké práce v zahraničných recenzovaných zborníkoch (AECA)</b>	<b>0 / 0</b>
<b>15. Publikované príspevky na domácich vedeckých konferenciách (AFB, AFD)</b>	<b>1 / 0</b>
<b>16. Publikované príspevky na zahraničných vedeckých konferenciách (AFA, AFC)</b>	<b>4 / 0</b>
<b>17. Vydané periodiká evidované v CCC, WoS Core Collection, SCOPUS</b>	<b>0</b>
<b>18. Ostatné vydané periodiká</b>	<b>0</b>
<b>19. Zostavovateľské práce knižného charakteru (FAI)</b>	<b>0 / 0</b>
<b>20. Preklady vedeckých a odborných textov (EAJ)</b>	<b>0 / 0</b>
<b>21. Heslá v odborných terminologických slovníkoch a encyklopédiách (BDA, BDB)</b>	<b>0 / 0</b>
<b>22. Recenzie v časopisoch a zborníkoch (EDI)</b>	<b>0 / 0</b>

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

Tabuľka 2f Štatistika vedeckých prác podľa kvartilu vedeckého časopisu

<b>Kvartil vedeckého časopisu</b>	<b>Q1</b>	<b>Q2</b>	<b>Q3</b>	<b>Q4</b>	<b>Spolu</b>
<b>Podľa IF z r. 2020 (zdroj JCR)</b>					
<i>Počet článkov / doplnky</i>	49 / 0	29 / 0	4 / 0	2 / 0	84 / 0
<b>Podľa SJR z r. 2020 (zdroj Scimago)</b>	48 / 0	19 / 0	17 / 0	1 / 1	85 / 1

Počet článkov / doplnky					
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Tabuľka 2g Ohlasy

OHLASY	Počet v r. 2020/ doplnky z r. 2019
Citácie vo WOS (1.1, 2.1)	1562 / 5
Citácie v SCOPUS (1.2, 2.2)	16 / 0
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	37
Prednášky a vývesky na národných vedeckých podujatiach	41

## 2.6. Vyžiadané prednášky

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

### 2.6.1. Vyžiadané prednášky na medzinárodných vedeckých podujatiach

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

KOMOROVSKÝ, S. Prediction of spectroscopic parameters for paramagnetic species containing heavy elements: Can the relativistic DFT methods do the job? Workshop Paramagnetic NMR in f elements, Toulouse, Francúzsko, 21.11. – 24.11. 2021

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

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

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

### 2.6.2. Vyžiadané prednášky na národných vedeckých podujatiach

### 2.6.3. Vyžiadané prednášky na významných vedeckých inštitúciách

PRNOVÁ, A. - PLŠKO, A. - VALÚCHOVÁ, J. - PECUŠOVÁ, B. - MAJEROVÁ, M. - KLEMENT, R. - GALUSEK, D. Termická analýza hlinitanových skiel, Univerzita Pardubice, Pardubice, Česká republika, 23. 9. 2021

## 2.7. Patentová a licenčná činnosť na Slovensku a v zahraničí v roku 2021

### 2.7.1. Vynálezy, na ktoré bol v roku 2021 udelený patent

a) na Slovensku

b) v zahraničí

### 2.7.2. Vynálezy prihlásené v roku 2021

a) na Slovensku

b) v iných krajinách ako prioritná prihláška

c) PCT

d) EP

e) v iných krajinách v rámci tzv. národnej fázy po PCT, resp. po validácii EP

**2.7.3. Úžitkové vzory na Slovensku**

a) prihlásené v roku 2021

b) udelené v roku 2021

**2.7.4. Realizované vynálezy**

a) predané patenty resp. prihlášky vynálezov (v prípade úplnej zmeny majiteľa patentu)

b) predané licencie (v prípade že majiteľom ostáva organizácia SAV)

*Finančný prínos pre organizáciu SAV v roku 2021 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
Boča Miroslav	VEGA	2
Korenko Michal	APVV	2
Prnová Anna	VEGA	1
Tatarko Peter	APVV-SK-SRB-21	4
	APVV-SK-UA-21	2
	VEGA-21	2

**2.9. Účasť na spracovaní hesiel do encyklopédie Beliana**

Počet autorov hesiel: 0

**2.10. Recenzovanie knižných publikácií a príspevkov vo vedeckých časopisoch**

Tabuľka 2j Počet vypracovaných recenzií na vedecké monografie, vedecké štúdie a zborníky

Meno pracovníka	Ved. monografie		Príspevky v časopisoch			Zborníky	
	Domáce	Zahra-ničné	WoS, SCOPUS	Iné databázy	Ostatné	Domáce	Zahra-ničné
Boča Miroslav	0	0	2	0	0	0	0
Bučko Tomáš	0	0	7	0	0	0	0
Bujdák Juraj	0	0	3	0	0	0	0

Galusek Dušan	0	0	24	0	0	0	0
Hanzel Ondrej	0	0	4	0	0	0	0
Kubíková Blanka	0	0	1	0	0	0	0
Lenčes Zoltán	0	0	14	0	0	0	0
Pálková Helena	0	0	2	0	0	0	0
Tatarko Peter	0	0	38	0	0	0	0
<b>Spolu</b>	<b>0</b>	<b>0</b>	<b>95</b>	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>

## 2.11. Iné informácie k vedeckej činnosti.

Počet časopiseckých karentovaných publikácií registrovaných v databáze WOS a Scopus v roku 2021 dosiahol číslo 80. V porovnaní s predchádzajúcim rokom počet publikačných výstupov narástol. V závislosti na metodike, na ktorú kategóriu sa vzťahuje 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 v danom roku. Na rok 2021 je tento počet 43,09 (a na jedného pracovníka pripadá 1,86 karentovanej publikácie. Po prirátaní deviatich doktorandov s plnou kapacitou (štyria ďalší doktorandi s kapacitou pod 0,3 vzhľadom na ich neskorší dátum nástupu na štúdium neboli zarátaní) sa počet VŠ zamestnancov zvýši na 52,09 počet publikácií na jedného pracovníka klesne na 1,54. Cieľom aj naďalej ostáva dosiahnuť dve publikácie na počet zamestnancov s univerzitným titulom zapojených do výskumných projektov, čo odpovedá štandardu vyspelých vedeckých pracovísk s podobným zameraním. Priemerný impakt faktor CCC časopisov, v ktorých boli práce uverejnené, bol 4,32, pokiaľ vlni to bolo 4,17 (treba mať na pamäti, že údaje sú zo záverečných správ, v ktorých sa nachádzajú aj doplnky publikácií za predchádzajúci rok 2020, ktorým ešte neboli priradené kompletne bibliografické údaje v čase spracovávaní podkladov do záverečných správ). Okrem CCC publikácií, vedeckí pracovníci ÚACH sa podieľali ako autori alebo spoluautori na dvoch kapitolách, ktoré vyšli v zahraničných nakladateľstvách.

Citovanosť (vo všetkých dostupných databázach WOS – 1567, SCOPUS – 16) na vedeckého pracovníka (37,3) je 42,0 citácií, čo predstavuje mierny nárast v porovnaní s rokom 2020. Pracovníci ústavu predniesli 5 pozvaných prednášok na významných medzinárodných konferenciách. Tento stav bol samozrejme ovplyvnený pandémiou.

Významnou časťou vedeckej aktivity je účasť na výzvach v rôznych projektových schémach. Z domácich projektov sa zaznamenala významná aktivita pri podávaní APVV projektov, ako vo všeobecnej výzve, tak aj v bilaterálnych výzvach (s Ruskom, Českou republikou, Srbskom a Čínou). Snahou je zvýšiť počet riešených projektov na ústave na úroveň roku 2019.

V 2021 boli podané dva projekty v rámci výzvy SASPRO 2 (1x v rámci schémy Incoming, 1x v rámci Reintegrácia). Jeden z nich bol medzinárodnou komisiou schválený na financovanie. Projekt začína v roku 2022. Ústav má aj ďalšieho úspešného uchádzača v rámci podpornej schémy pre post-doktorandov - Schwarzov fond.

### 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 2021

Forma	Počet k 31.12.2021				Počet doktorandov po doktorandskej skúške		Počet ukončených doktorantúr v r. 2021					
							Ukončenie z dôvodov					
	celkový počet		z toho novoprijatí				ukončenie úspešnou obhajobou		predčasné ukončenie		neúspešné ukončenie	
M	Ž	M	Ž	M	Ž	M	Ž	M	Ž	M	Ž	
Denná zo zdrojov SAV	7	6	3	1	6	3	3	0	0	0	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	0	0	0	0	0	0
Spolu	7	6	3	1	6	3	3	0	0	0	0	0
Z toho zahraničných	6	4	2	1	4	1	1	0	0	0	0	0
Súhrn	13		4		9		3		0		0	

Uvádzajte len doktorandov organizácie ako externej vzdelávacej inštitúcie.

Riadok „Spolu“ je súčtom troch riadkov nad ním. Každá bunka v riadku „Súhrn“ vyjadruje celkový počet doktorandov (mužov a žien spolu), čiže je súčtom príslušných dvoch buniek z riadku „Spolu“. V stĺpci „Počet doktorandov po doktorandskej skúške“ sa uvádza počet doktorandov, ktorí počas roku 2021 boli aspoň 1 deň doktorandami po doktorandskej skúške. Sú číselne zahrnutí aj v predchádzajúcich stĺpcoch.

Pod predčasným ukončením rozumieme ukončenie bez obhajoby dizertačnej práce pričom doktorand neabsolvoval celú štandardnú dĺžku štúdia. Pod neúspešným ukončením rozumieme ukončenie bez úspešnej obhajoby dizertačnej práce, pričom študent absolvoval celú štandardnú dĺžku štúdia.

#### 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 2021 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 hodnotu
Ing. Martin Barlog	interné štúdium hraené z	9 / 2017	8 / 2021	5.2.19 anorganická technológia a materiály	Ing. Helena Páľková PhD., Ústav anorganickej	Fakulta chemickej a potravinárskej technológie STU

	prostriedkov SAV				chémie SAV	
Daniel Moreno Rodriguez	interné štúdium hradené z prostriedkov SAV	9 / 2017	8 / 2021	5.2.19 anorganická technológia a materiály	Ing. Eva Scholtzová CSc., Ústav anorganickej chémie SAV	Fakulta chemickej a potravinárskej technológie STU

### 3.4. Zoznam doktorandov, ktorí ukončili doktorandské štúdium úspešnou obhajobou v nadštandardnej dĺžke štúdia

Tabuľka 3d Menný zoznam ukončených doktorandov v roku 2021 úspešnou obhajobou v nadštandardnej dĺžke štúdia

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
Ing. Michal Hičák	interné štúdium hradené z prostriedkov SAV	2 / 2015	8 / 2021	4.1.15 anorganická chémia	prof. RNDr. Pavol Šajgalík DrSc., Ústav anorganickej chémie SAV	Prírodovedecká fakulta UK

### 3.5. Uplatnenie absolventov doktorandského štúdia

Tabuľka 3e Prehľad uplatnenia absolventov doktorandského štúdia

Počet absolventov PhD. štúdia v roku 2021 (obhajoba leto 2021)	z toho koľkí sa zamestnali vo výskume (SAV, univerzity, rezortné výskumné ústavy)	z toho koľkí sa zamestnali v praxi mimo výskum, kde využívajú svoju kvalifikáciu	z toho koľkí sa zamestnali v praxi, kde nevyužívajú svoju kvalifikáciu	z toho koľkí boli nejaký čas nezamestnaní
3	3	0	0	0

Zoznam interných a externých doktorandov je uvedený v prílohe A.

### 3.6. Medzinárodné doktorandské štúdium

Tabuľka 3f Počet študentov v medzinárodných programoch doktorandského štúdia

Cotutelle	Co-direction	Iné	Zahraniční doktorandi štátne občianstvo/počet
0	0	0	IND/2, TUR/2, DEU/1, ECU/1, ESP/1, GRC/1, IRN/1, PAK/1, RUS/1

Zahraniční doktorandi sú doktorandi v dennej alebo externej forme štúdia, ktorí sú občanmi iných krajín.

Doktorandi školení v rámci Cotutelle alebo Co-direction sa do posledného stĺpca nezapočítavajú.

### 3.7. Zoznam študijných odborov, na ktoré má ústav uzatvorenú rámcovú dohodu, s uvedením VŠ

Tabuľka 3g Zoznam študijných odborov, na ktoré má ústav uzatvorenú rámcovú dohodu, s uvedením univerzity/vysokej školy a fakulty, kde sa doktorandský študijný program uskutočňuje

Názov študijného odboru (ŠO)	Číslo ŠO	Názov doktorandského študijného programu	Doktorandské štúdium uskutočňované na (univerzita/vysoká škola a fakulta)
chémia	1420	anorganická chémia	PríF UK/FCHPT STU
chémia	1420	fyzikálna chémia	PríF UK/FCHPT STU
chémia	1420	teoretická a počítačová chémia	PríF UK
fyzika	1160	chemická fyzika	PríF UK
chemické inžinierstvo a technológie	2820	anorganická technológia a materiály	FCHPT STU/TnUAD

Názov a číslo študijného odboru vyplňte/vyberte podľa aktuálne platného zoznamu študijných odborov <https://www.portalvs.sk/sk/studijne-odbory?from=menu1>.

Do 31. 8. 2023 študujú študenti doktorandského štúdia zaradení do študijných programov podľa zoznamu MŠVVaŠ, platného do 1. 9. 2019. Pre týchto študentov je potrebné napísať názov programu ako voľný text do stĺpca 3.

Tabuľka 3h Účasť na pedagogickom procese

Menný prehľad pracovníkov, ktorí boli menovaní do 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. (Fakulta chemickej a potravinárskej technológie STU)	Ing. Jarmila Mlynáriková, PhD. (IIa)
doc. Ing. Miroslav Boča, DrSc. (anorganická technológia a materiály)	doc. Ing. Miroslav Boča, DrSc. (Trenčianska univerzita Alexandra Dubčeka v Trenčíne)	Mgr. Jan Novotný, PhD. (IIa)
doc. Ing. Miroslav Boča, DrSc. (odbor v zahraničí)	prof. Ing. Dušan Galusek, DrSc. (Fakulta špeciálnej techniky TnUAD)	
prof. RNDr. Juraj Bujdák, DrSc. (anorganická chémia)	prof. Ing. Dušan Galusek, DrSc. (Fakulta zdravotníctva TnUAD)	
prof. 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., Dr.h.c. (Fakulta chemické technológie VŠCHT, Praha, ČR)	
prof. Ing. Dušan Galusek, DrSc.	prof. Ing. Marek Liška, DrSc.,	

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



### 3.8. Údaje o pedagogickej činnosti

Tabuľka 3i Prednášky a cvičenia vedené v roku 2021

PEDAGOGICKÁ ČINNOSŤ	Prednášky		Cvičenia a semináre	
	doma	v zahraničí	doma	v zahraničí
Počet prednášateľov alebo vedúcich cvičení	3	1	1	0
Celkový počet hodín v r. 2021	83	32	52	0

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

Tabuľka 3j Aktivity pracovníkov na VŠ

1.	Počet pracovníkov, ktorí pôsobili ako vedúci alebo konzultanti diplomových a bakalárskych prác	0
2.	Počet vedených alebo konzultovaných diplomových a bakalárskych prác	0
3.	Počet pracovníkov, ktorí pôsobili ako školitelia doktorandov (PhD.)	15
4.	Počet školených doktorandov (aj pre iné inštitúcie)	28
5.	Počet oponovaných dizertačných a habilitačných prác	13
6.	Počet pracovníkov, ktorí oponovali dizertačné a habilitačné práce	6
7.	Počet pracovníkov, ktorí pôsobili ako členovia komisií pre obhajoby DrSc. prác	2
8.	Počet pracovníkov, ktorí pôsobili ako členovia komisií pre obhajoby PhD. prác	6
9.	Počet pracovníkov, ktorí pôsobili ako členovia komisií, resp. oponenti v inauguračnom alebo habilitačnom konaní na vysokých školách	1

### 3.9. Iné dôležité informácie k pedagogickej činnosti

Ústav anorganickej chémie SAV bol začiatkom roka vyzvaný fakultami vysokých škôl, s ktorými má podpísanú dohodu o spolupráci v oblasti doktorandského štúdia, na vypísanie tém pre tretí stupeň štúdia. Celkovo bolo vypísaných 16 tém v troch študijných programoch (anorganická chémia a fyzikálna chémia v spolupráci s PríF UK a anorganická technológia a materiály v spolupráci s FCHPT STU). Tieto témy boli zverejnené aj na ďalších dvoch medzinárodných portáloch, ako vlastná iniciatíva ÚACH SAV pre získanie nových doktorandov. Piaty zo siedmich záujemcov sa zúčastnili prijímacích pohovorov. Zo štyroch úspešných uchádzačov nastúpili všetci štyria študenti a boli zapísaní do prvého ročníka doktorandského štúdia na PríF UK v programe Anorganická chémia (3 zahraniční študenti) a na FCHPT STU v programe anorganická technológia a materiály (1 študent zo Slovenska). Študenti doktorandského štúdia a mladí vedeckí pracovníci do 35 rokov sa po ročnej prestávke zapríčinené zlou pandemickou situáciou na jeseň v minulom roku, zapojili do Súťaže mladých pracovníkov do 35 rokov na ÚACH SAV. Súťaž sa uskutočnila 5.10.2021 za účasti 12 študentov doktorandského štúdia z ÚACH SAV Bratislava a TnUAD Trenčín. Na ocenených miestach sa umiestnili:

1. Hakan Ünsal
2. Debora Mišenkova a Nurshen Mutlu
3. Florian Lemken

Doktorandi ÚACH sa uchádzajú aj o projekty v rámci výziev DOKTOGRANT, v roku 2021 sa o tento projekt úspešne uchádzala doktorandka Eva Skoura. Doktorand Florian Lemken sa uchádzal o grant Francúzskeho inštitútu na Slovensku a Ministerstva školstva, vedy výskumu a športu SR, ktorý slúži v rámci programu na podporu vedeckej aktivity mladých vedeckých pracovníkov, ktorí pracujú na Slovensku.

## 4. Medzinárodná vedecká spolupráca

### 4.1. Medzinárodné vedecké podujatia

#### 4.1.1. Medzinárodné vedecké podujatia, ktoré organizácia SAV organizovala v roku 2021 alebo sa na ich organizácii podieľala, s vyhodnotením vedeckého a spoločenského prínosu podujatia

**XIV. workshop o moderných metódach v kvantovej chémii**, online konferencia, Bratislava, Slovensko, 38 účastníkov, 01. - 03. 03.2021

Účastníci z Fínska, Nemecka, Nórska, Rakúska, Českej republiky, Slovenska, Francúzska. Na podujatí odznelo 15 prednášok

**14<sup>th</sup> International Conference on Solid State Chemistry**, Trenčín, Slovenská republika, 106 účastníkov, 13.06.-17.06.2021

UaCh ako spoluorganizátor, spolu so SSS, SSiS, SchS, Uni Pardubice, hlavný organizátor TnUAD, 106 účastníkov z 15 krajín, celkovo 65 prednášok, z toho 21 pozvaných a 13 postrov. Vybrané príspevky budú s podporou IUPAC zverejnené v špeciálnom čísle časopisu Pure and Applied Chemistry

#### 4.1.2. Medzinárodné vedecké podujatia, ktoré usporiada organizácia SAV v roku 2022 (anglický a slovenský názov podujatia, miesto a termín konania, meno, telefónne číslo a e-mail zodpovedného pracovníka)

**XV<sup>th</sup> Workshop on Modern Methods in Quantum Chemistry** /XV. workshop o moderných metódach v kvantovej chémii, Bratislava, Slovensko, 06.03.-11.03.2022, (Ol'ga Malkin, 02/59410422, uacholga@savba.sk)

**17<sup>th</sup> Conference on High Temperature Materials Chemistry (HTMC XVII)**, Horný Smokovec, Slovenská republika, 11.09.-16.09.2022, (Miroslav Boča, 02/59410400, uachboca@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	0	0	1
Galusek Dušan	0	0	1
Komorovský Stanislav	0	1	0
Malkin Ol'ga	0	0	1
<b>Spolu</b>	0	1	3

### 4.2. Členstvo a funkcie v medzinárodných orgánoch

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

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)

prof. RNDr. Juraj Bujdák, DrSc.

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

prof. Ing. Dušan Galusek, DrSc.

American Ceramic Society (funkcia: člen)  
Ceramic in Modern Technologies (funkcia: člen)  
European Ceramic Society (funkcia: člen)  
European Society for Bioresorbable Implants (funkcia: zakladajúci člen)  
European Society on Glass Science and Technology (funkcia: člen)

doc. Ing. Mária Chromčíková, PhD.

Česká sklárska spoločnosť (funkcia: člen)  
TC03 (funkcia: člen)

Mgr. Ľuboš Jankovič, PhD.

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

Ing. Michal Korenko, PhD.

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

Mgr. Valéria Kureková, PhD.

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

doc. Ing. Zoltán Lenččš, PhD.

American Ceramic Society (funkcia: člen)  
Ceramic Society of Japan (funkcia: člen)  
European Ceramic Society (funkcia: člen výboru)  
International Ceramic Federation (funkcia: člen)  
Materials Research Society (funkcia: člen)

prof. Ing. Marek Liška, DrSc., Dr.h.c.

Česká sklárska spoločnosť (funkcia: člen výboru, čestný člen)  
ICG TC03 (funkcia: člen)  
Society of Glass Technology (funkcia: čestný člen - FSGT)

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)

MSc. Daniel Moreno, PhD.

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

Ing. Helena Pálková, PhD.

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

Mgr. Marek Pribus, PhD.

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

Ing. Anna Prnová, PhD.

Slovak Fulbright Alumni Association (funkcia: člen)

Ing. Eva Scholtzová, CSc.

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

Ing. Michal Slaný, PhD.

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)

European Ceramic Society (funkcia: člen predstavenstva)

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)

Mgr. Tímea Šimonová, PhD.

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

Ing. Peter Škorňa, PhD.

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

#### 4.3. Účast' 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
Bučko Tomáš	DECI 17th project	1
Galusek Dušan	H2020 ERC consolidator grant	1
Korenko Michal	EUROATOM	1
Tatarko Peter	EU HORIZON-MSCA-2021-PF-01	6
	Latvian Science Fund / call for Fundamental and Applied Research	4
	Serbian Science Fund / IDEAS	1

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

**Miroslav Boča**

- ENEA Research center, Casaccia, Talianko (15. – 18. 11. 2021) v rámci riešenia projektu – Heat capacities of fluorozirconate compounds (SURPF2001310039) získaného v rámci európskeho projektu SFERA3 v roku 2020.

**Ondrej Hanzel**

- Vinča Institute of Nuclear Science, University of Belgrade, Srbsko (17.10. - 19.10.2021) - stretnutie riešiteľov a realizácia experimentov v rámci projektu APVV-SK-SRB-18-022.

**Blanka Kubíková**

- ENEA Research center, Casaccia, Talianko (15. – 26. 11. 2021) v rámci riešenia projektu – Heat capacities of fluorozirconate compounds (SURPF2001310039) získaného v rámci európskeho projektu SFERA3 v roku 2020.

**Helena Pálková**

- Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow, Poľsko, návšteva spolupracujúceho pracoviska s cieľom diskusie o ďalších možnostiach spolupráce a uskutočnenie meraní na pokročilých experimentálnych zariadeniach na vzorkách pripravených v rámci projektov riešených na ústave.

**Marek Pribus**

- Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow, Poľsko, návšteva spolupracujúceho pracoviska s cieľom diskusie o ďalších možnostiach spolupráce a uskutočnenie meraní na pokročilých experimentálnych zariadeniach na vzorkách pripravených v rámci projektov riešených na ústave.

**Eva Scholtzová**

- Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow, Poľsko, návšteva spolupracujúceho pracoviska s cieľom diskusie o ďalších možnostiach spolupráce.

**Peter Tatarko**

- Vinča Institute of Nuclear Science, University of Belgrade, Srbsko (17.10. - 19.10.2021) - stretnutie riešiteľov a realizácia experimentov v rámci projektu APVV-SK-SRB-18-022.
- Ústav fyziky materiálov, AVČR, Brno, Česká republika (25.10. - 27.10.2021) - stretnutie riešiteľov a realizácia experimentov v rámci projektu Mobility SAV-AVČR-21-04.
- Ústav fyziky materiálov, AVČR, Brno, Česká republika (22.11. - 23.11.2021) - stretnutie riešiteľov a realizácia experimentov v rámci projektu Mobility SAV-AVČR-21-04.

**Hakan Ünsal**

- Vinča Institute of Nuclear Science, University of Belgrade, Srbsko (17.10. - 19.10.2021) - stretnutie riešiteľov a realizácia experimentov v rámci projektu APVV-SK-SRB-18-022.
- Ústav fyziky materiálov, AVČR, Brno, Česká republika (25.10. - 27.10.2021) - stretnutie riešiteľov a realizácia experimentov v rámci projektu Mobility SAV-AVČR-21-04.
- Ústav fyziky materiálov, AVČR, Brno, Česká republika (22.11. - 23.11.2021) - stretnutie riešiteľov a realizácia experimentov v rámci projektu Mobility SAV-AVČR-21-04.

**Prednášky zahraničných hostí na ÚACH SAV v roku 2021****Dr. Dejan Zagorac** (Vinča Institute of Nuclear Science, University of Belgrade, Srbsko)

- Recent advances in materials research: structure prediction, novel methods and databases with connections to the experimental data, 29. 9. 2021

**prof. Branko Matovic** (Vinča Institute of Nuclear Science, University of Belgrade, Srbsko)

- Controllable synthesis of doped ceria nanopowders by cations with different valence state, 27. 9. 2021

**Dr. Ivana Cvijović – Alagić**

- Effect of severe plastic deformation processing on the Ti-45Nb alloy performance in physiological conditions, 27. 9. 2021

*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. Koncepcia dlhodobého rozvoja organizácie

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.

### 5.1. Odporúčania z posledného pravidelného hodnotenia organizácií SAV (akreditácie)

Uvádame odporúčania, ktoré sme dostali od hodnotiaceho panela.

- The numbers of publications in highly cited international journals should be further increased.
- More university lectures could help to increase the interest of PhD students in the subject.
- The institute should aim at more funding at the EU level.
- Further possible connections to commercial applications should be explored.

Ako je vidieť sú to pomerne všeobecné formulácie. Aj napriek tomu sú tieto odporúčania podrobne rozpracované v akčnom pláne spolu s cieľovými hodnotami v rôznych časových horizontoch v závislosti od problematiky.

### 5.2. Hlavné body Akčného plánu organizácie a stav ich plnenia

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.

### **Technická infraštruktúra**

Neoddeliteľnou súčasťou vednej politiky je aj rozvoj infraštruktúry. Ústav cielene buduje svoju infraštruktúru na rôznych úrovniach cez laboratória 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.

### **5.3. Aktualizácia Akčného plánu organizácie v roku 2021**

Diskusie o akčnom pláne ústavu sú obojstranný problém. Je to dokument živý, ktorý si vyžaduje konkrétne zmeny v závislosti na okolnostiach (napr. zmeny v grantových agentúrach, legislatívne zmeny, prípadne zmeny a zámery zo strany P SAV). Na jednej strane je snaha naplňovať zadané ciele a ukazovatele zo strany ústavu, na strane druhej očakávame aj aktivity zo strany P SAV na podnety ústavu/ústavov. Ako príklad možno uviesť absenciu projektového oddelenia. Netreba tento problém rozpisovať, lebo všetci vieme aká má byť jeho úloha, ako má fungovať atď. Treba ho iba zriadiť.



## 6. Spolupráca s univerzitami/vysokými školami a inými subjektmi v oblasti vedy a techniky, okrem aktivít uvedených v kap. 2, 3, 4

### 6.1. Spoločné pracoviská organizácie

#### 6.1.1. Spolupráca s univerzitami/VŠ (fakultami)

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

**Oblasť spolupráce:** vedecká spolupráca, účasť na PhD. výuke

**Sídlo spoločného pracoviska (ak je vytvorené):**

**Začiatok spolupráce:** 1990

**Zhodnotenie:** Ústav je zapojený do vzdelávania na III. stupni vysokoškolského štúdia v študijných programoch „Anorganická chémia“, „Fyzikálna chémia“ a „Anorganická technológia a materiály“. Pracovníci ÚACh viedli na FChPT v roku 2021 dvoch doktorandov, ktorí v auguste úspešne obhájili predložené dizertačné práce. Doc. Ing. Miroslav Boča, DrSc. je navyše členom odborej komisie pre študijný program Anorganická technológia a materiály a externým členom VR FCHPT STU.

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

**Oblasť spolupráce:** vedecká spolupráca, účasť na Bc. a Mgr. výuke

**Sídlo spoločného pracoviska (ak je vytvorené):**

**Začiatok spolupráce:** 2000

**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:** Montanuniversitaet Leoben, Rakúsko

**Oblasť spolupráce:** vedecká spolupráca, výchova doktorandov

**Sídlo spoločného pracoviska (ak je vytvorené):**

**Začiatok spolupráce:** 2008

**Zhodnotenie:** Spolupráca je zameraná na výchovu mladých doktorandov so zameraním na pokročilé žiaruvzdorné keramické materiály. Prof. RNDr. P. Šajgalík, DrSc. a doc. Ing. Z. Lenčes, PhD. sú školiteľmi špecialistami doktorandov.

**Názov univerzity/vysokej školy a fakulty:** Prírodovedecká fakulta UK

**Oblasť spolupráce:** vedecká spolupráca, účasť na Bc., Mgr. a PhD. výuke

**Sídlo spoločného pracoviska (ak je vytvorené):**

**Začiatok spolupráce:** 1990

**Zhodnotenie:** V spolupráci s touto fakultou je ústav zapojený do vzdelávania na III. stupni vysokoškolského štúdia v študijných programoch „Anorganická chémia“, „Fyzikálna chémia“ a „Chemická fyzika“. V roku 2021 bol podpísaný dodatok k rámcovej zmluve o spolupráci na doktorandskom štúdiu, ktorého obsahom bolo rozšírenie študijných programov, na ktorých sa ÚACH SAV môže podieľať o študijných program „Teoretická a počítačová chémia“. Spoločne sa riešia projekty VEGA a APVV. prof. RNDr. J. Bujdák, DrSc. má hlavný úväzok na fakulte a čiastkový na ÚACH SAV. Prof. RNDr. J. Bujdák, DrSc. je interným členom VR ústavu a RNDr. Jana Madejová, DrSc. externým členom VR PriF UK. Pracovníci ÚACh viedli na PriF UK v priebehu roka 2021 13 doktorandov, pričom jeden z nich v auguste 2021 štúdium úspešne ukončil obhajobou svojej práce.

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

**Oblasť spolupráce:** vedecká spolupráca, účasť na výchove doktorandov

**Sídlo spoločného pracoviska (ak je vytvorené):** Centrum kompetencie pre výskum skla Vitrum Laugaricio v Trenčíne

**Začiatok spolupráce:** 1997

**Zhodnotenie:** Okrem spoločného pracoviska s TnU AD (Centrum kompetencie skla Vitrum Laugaritio) rieši ÚACH SAV v spolupráci s touto univerzitou spoločné projekty VEGA a APVV. Prof. Ing. D. 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). Pracovníci centra, zamestnanci ÚACH, sa

podieľajú na pedagogickej činnosti v rámci doktorandského štúdia v odbore "Anorganická technológia". Od roku 2019 má ÚACh SAV s TnU AD rámcovú dohodu o spolupráci pri uskutočňovaní doktorandského študijného programu v odbore 5.2.19 Anorganická technológia a materiály.

**Názov univerzity/vysokej školy a fakulty:** Ukrainian State University of Chemical Technology, Dnipro, Ukraine

**Oblasť spolupráce:** vedecká spolupráca

**Sídlo spoločného pracoviska (ak je vytvorené):**

**Začiatok spolupráce:** 2018

**Zhodnotenie:** Vedecká spolupráca pri analýzach povrchov kovových materiálov upravených elektrochemickým leštením sa v roku 2021 zamerala na skúmanie vlastností takto pripravených materiálov a spoločné publikácie.

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

**Oblasť spolupráce:** príprava keramických a sklokeramických materiálov v systémoch  $\text{Al}_2\text{O}_3\text{-La}_2\text{O}_3$ ,  $\text{Al}_2\text{O}_3\text{-La}_2\text{O}_3\text{-ZrO}_2$ ,  $\text{Al}_2\text{O}_3\text{-Y}_2\text{O}_3$

**Sídlo spoločného pracoviska (ak je vytvorené):**

**Začiatok spolupráce:** 2010

**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. Vedecká spolupráca pri príprave amorfných a polykryštalických materiálov sol-gel metódami v systémoch  $\text{Al}_2\text{O}_3\text{-La}_2\text{O}_3$ ,  $\text{Al}_2\text{O}_3\text{-La}_2\text{O}_3\text{-ZrO}_2$ ,  $\text{Al}_2\text{O}_3\text{-Y}_2\text{O}_3$ .

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

**Oblasť spolupráce:** vedecká spolupráca, výchova doktorandov

**Sídlo spoločného pracoviska (ak je vytvorené):**

**Začiatok spolupráce:** 2010

**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. Lenčes, PhD. je členom odborovej rady doktorandského študijného programu Materiálové vedy a inžinýrství.

*Pozn.: uvádzajte len tie spolupráce, na ktoré má organizácia zmluvu resp. memorandum o zriadení spoločného pracoviska, resp. o vzájomnej spolupráci v konkrétnej oblasti výskumu*

### 6.1.2. Spoločné pracoviská s inými organizáciami SAV

**Názov organizácie:** Ústav vied o Zemi SAV

**Oblasť spolupráce:** vedecká spolupráca

**Sídlo spoločného pracoviska (ak je vytvorené):** Banská Bystrica

**Začiatok spolupráce:** 2018

**Zhodnotenie:** Podaný spoločný projekt vo výzve OPVaI-VA/DP/2018/1.2.1-05. Medzi ústavom a ÚVZ SAV je uzatvorená zmluva o spolupráci na dobu neurčitú, keďže sa aj v budúcnosti predpokladá podávanie spoločných projektov.

*Pozn.: uvádzajte len tie spolupráce, na ktoré má organizácia zmluvu resp. memorandum o zriadení spoločného pracoviska, resp. o vzájomnej spolupráci v konkrétnej oblasti výskumu*

### 6.2. Spoločné pracoviská organizácie s inými inštitúciami mimo SAV a VŠ

*Pozn.: uvádzajte len tie spolupráce, na ktoré má organizácia zmluvu resp. memorandum o zriadení spoločného pracoviska, resp. o vzájomnej spolupráci v konkrétnej oblasti výskumu*

### 6.3. Spoločné projekty s univerzitami a ostatnými inštitúciami mimo SAV

*Pozn.: uviesť konkrétne spoločné aj bilaterálne projekty na základe platnej zmluvy o spolupráci*

### 6.4. Iné typy spoločných aktivít s inštitúciami mimo SAV

## **7. Aplikácia výsledkov výskumu v spoločenskej a hospodárskej praxi**

### **7.1. Výsledky výskumu organizácie aplikované v spoločenskej a hospodárskej praxi**

#### **7.2. Kontraktový – zmluvný výskum (vrátane zahraničných kontraktov)**

Názov/účel kontraktového výskumu: Consultation service to transfer electrochemical method in lab at Voreppe in France

Zadávateľ výskumného kontraktu: Rio Tinto Aluminium Pechiney, Francúzsko

Začiatok spolupráce: 2021

Ukončenie spolupráce: trvá

Finančný prínos pre organizáciu (€): 4500

Názov/účel kontraktového výskumu: Dissolution rate of 4 different aluminas

Zadávateľ výskumného kontraktu: Rio Tinto Aluminium Pechiney, Francúzsko

Začiatok spolupráce: 2021

Ukončenie spolupráce: trvá

Finančný prínos pre organizáciu (€): 0

#### **7.3. Iné formy aplikácie výsledkov výskumu v spoločenskej a hospodárskej praxi**

## 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
doc. Ing. Miroslav Boča, DrSc.	Komisia pre obhajoby doktorských dizertačných prác v odbore anorganická chémia - 01402	predseda
prof. Ing. Dušan Galusek, DrSc.	Ad hoc komisia pre obhajoby doktorských dizertačných prác v odbore Anorganická technológia a materiály	predseda
	Slovenská komisia pre vedecké hodnosti	člen
Ing. Michal Korenko, PhD.	Komisia pre námietky pri verejnom obstarávaní	externý člen
doc. Ing. Zoltán Lenčoš, PhD.	Sektorová rada inovácií, Národná sústava povolaní	člen
prof. RNDr. Pavol Šajgalík, DrSc.	Výskumná agentúra SR	člen
	Pandemická komisia MZ SR	člen
	Rada predsedov pracovných skupín pre prioritné oblasti aplikovaného výskumu a experimentálneho vývoja	predseda
	Komisia ministra školstva pre udeľovanie Ceny ministra školstva	člen
	Technologická agentúra SR	člen
	Slovenská komisia pre vedecké hodnosti (SKVH)	podpredseda
	Rada vlády pre vedu, techniku a inovácie	podpredseda
	Komisia MŠ pre prioritné oblasti aplikovaného výskumu a experimentálneho vývoja v SR - materiálový výskum a nanotechnológie	člen pracovnej skupiny

### 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 vládnymi 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	0	tlač	0	TV	2
rozhlas	1	internet	1	exkurzie	1
publikácie	1	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
XIV. workshop o moderných metódach v kvantovej chémii, online konferencia	medzinárodná	Bratislava, Slovensko	01.03.-03.03.2021	38
14th International Conference on Solid State Chemistry	medzinárodná	Trenčín, Slovenská republika	13.06.-17.06.2021	106

### 9.3. Účasť na výstavách

Názov výstavy: Európska Noc Vyskumníkov 2021

Miesto konania: On-line

Dátum: 24.9.2021

Zhodnotenie účasti: V rámci podaktivity "Navštív svoju školu - Spoznaj svojho vedca" boli uskutočnené dve prednášky (P. Boháč) na školách Základná škola Zarevúca v Ružomberku a Gymnázium v Ružomberku.

### 9.4. Účasť v programových a organizačných výboroch národných konferencií

Tabuľka 9c Programové a organizačné výbory národných konferencií

Meno pracovníka	Programový	Organizačný	Programový i organizačný
Bujdák Juraj	0	0	1
Galusek Dušan	0	0	1
Páľková Helena	0	0	1
Šimonová Tímea	0	1	0
<b>Spolu</b>	0	1	3

### 9.5. Členstvo v redakčných radách časopisov

doc. Ing. Miroslav Boča, DrSc.

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

prof. 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)  
International Journal of Applied Ceramic Technology (funkcia: associate editor)  
Journal of the European Ceramic Society (funkcia: editor)  
New Journal of Glass and Ceramics (funkcia: člen)

doc. Ing. Zoltán Lenčoš, PhD.

International Journal of Applied Ceramic Technology (funkcia: člen)  
Journal of the Ceramic Society of Japan (funkcia: associate editor)

prof. Ing. Marek Liška, DrSc., Dr.h.c.

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)

Ing. Peter Tatarko, PhD.

International Journal of Applied Ceramic Technology (funkcia: associate editor)  
Materials (funkcia: editorial board member)

**9.6. Činnosť v domácich vedeckých spoločnostiach**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)

prof. 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)

prof. Ing. Dušan Galusek, DrSc.

Humboldtov klub v SR (funkcia: člen)  
Slovenská silikátová vedecko-technická spoločnosť (funkcia: podpredseda)  
Slovenská sklárska spoločnosť (funkcia: predseda (od 11/2021))  
Slovenská sklárska spoločnosť (funkcia: člen predstavenstva, vedecký tajomník)

doc. Ing. Miroslav Hnatko, PhD.

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

doc. Ing. Mária Chromčíková, PhD.

Slovenská akreditačná spoločnosť pre vysoké školy (funkcia: člen)  
Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)  
Slovenská sklárska spoločnosť (funkcia: člen)

Mgr. Ľuboš Jankovič, PhD.

Slovenská ílová spoločnosť (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)

Mgr. Valéria Kureková, PhD.

Slovenská chemická spoločnosť (funkcia: člen)  
Slovenská ílová spoločnosť (funkcia: člen)

doc. Ing. Zoltán Lenčoš, PhD.

Humboldtov klub v SR (funkcia: člen)  
Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen výboru)

prof. Ing. Marek Liška, DrSc., Dr.h.c.

Slovenská chemická spoločnosť (funkcia: člen)  
Slovenská sklárska spoločnosť (funkcia: člen)

RNDr. Jana Madejová, DrSc.

Slovenská chemická spoločnosť (funkcia: člen)  
Slovenská ílová spoločnosť (funkcia: člen)  
Učená spoločnosť SAV (funkcia: člen)

Dr. Vladimír Malkin, DrSc.

Humboldtov klub v SR (funkcia: člen)

Ing. Monika Micháľková, PhD.

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)  
Slovenská sklárska spoločnosť (funkcia: členka predstavenstva, tajomníčka od 22.10.2021)

Ing. Jarmila Mlynáriková, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

MSc. Daniel Moreno, PhD.

Slovenská ílová spoločnosť (funkcia: člen)

Ing. Zuzana Netriová, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

Ing. Helena Pálková, PhD.

Slovenská ílová spoločnosť (funkcia: podpredseda)

Ing. Viliam Pavlík, PhD.

Slovenská chemická spoločnosť (funkcia: člen)  
Slovenská nukleárna spoločnosť (funkcia: člen)

Mgr. Marek Pribus, PhD.

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)

RNDr. Veronika Siliková, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

Ing. Michal Slaný, PhD.

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)

Mgr. Tímea Šimonová, PhD.

Slovenská ílová spoločnosť (funkcia: člen)

Ing. Peter Škorňa, PhD.

Slovenská ílová spoločnosť (funkcia: člen)

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****Letná škola mladých vedcov**

Ústav anorganickej chémie sa prostredníctvom Ing. Viliam Pavlíka, PhD. zapojil do Letnej školy mladých vedcov organizovanej občianskym združením All4Science. Na jeden týždeň si žiaci prvého a druhého stupňa základných škôl mali možnosť vyskúšať, aké je to pracovať v laboratóriu a myslieť ako vedec. Na programe boli zaujímavé experimenty, ako napríklad vplyv tekutého dusíka na správanie rôznych materiálov, alebo tavenie a vylievanie špeciálneho skla pri 1500 °C. Nechýbala výroba "zápalnej zmesi", ktorá sa následne použila do vopred zhotovených malých rakiet. Po niekoľkých neúspešných pokusoch a úprave dizajnu rakiet, sa žiakom úspešne podarilo vyštartovať k nebesám so slovami "päť sekúnd - let normálny". Na záver týždňa si žiaci pripravili papierové vývesky, aby prezentovali svoju prácu pred žiakmi, ktorí boli na iných ústavoch.



## 10. Činnosť knižnično-informačného pracoviska

### 10.1. Knižničný fond

Tabuľka 10a Knižničný fond

<b>Knižničné jednotky spolu</b>		7636
z toho	knihy a zviazané periodiká	7636
	audiovizuálne dokumenty	
	elektronické dokumenty (vrátane digitálnych)	1
	mikroformy	
	iné špeciálne dokumenty - dizertácie, výskumné správy	
	Rukopisy, vzácne tlače	
Počet titulov dochádzajúcich periodík		
z toho zahraničné periodiká		
Ročný prírastok knižničných jednotiek		7
v tom	kúpou	7
	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

<b>Výpožičky spolu (riadok 1)</b>		
v tom z r. 1	prezenčné výpožičky	
	absenčné výpožičky	
v tom z r. 1	odborná literatúra pre dospelých	
	výpožičky periodík	
MVS iným knižniciam		
MVS z iných knižníc		
MMVS iným knižniciam		
MMVS z iných knižníc		
Počet vypracovaných bibliografií		
Počet vypracovaných rešerší		49

### 10.3. Používatelia

Tabuľka 10c Používatelia

Registrovaní používatelia	
Návštevníci knižnice spolu (bez návštevníkov podujatí)	

**10.4. Iné údaje**

Tabuľka 10d Iné údaje

On-line katalóg knižnice na internete ( 1=áno, 0=nie)	
Náklady na nákup knižničného fondu v €	986,61

**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 v komisiách SAV

doc. Ing. Miroslav Boča, DrSc.

- Komisia SAV pre informačné a komunikačné technológie (člen)
- Komisia SAV pre posudzovanie vedeckej kvalifikácie zamestnancov (člen)
- Komisia SAV pre vyhodnocovanie medzinárodných projektov (člen)

Ing. Michal Korenko, PhD.

- Komisia pre hodnotenie grantov doktorandov SAV (člen)

### 11.4. Členstvo v orgánoch VEGA

prof. Ing. Dušan Galusek, DrSc.

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

Mgr. Stanislav Komorovský, PhD.

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

## 12. Hospodárenie organizácie

### 12.1. Výdavky organizácie

Tabuľka 12a Výdavky organizácie (skutočnosť k 31. 12. 2021 v €)

Typ organizácie (RO,PO)		Zdroje, z ktorých sa kryli jednotlivé výdavky			
Výdavky	Spolu	kapitola SAV (111)	iné štátne a verejné zdroje	ostatné zdroje	% krytia z kapitoly SAV
<b>1. Bežné výdavky</b>	<b>2 383 812</b>	<b>1 724 046</b>	<b>545 359</b>	<b>114 407</b>	<b>72</b>
z toho: mzdy (610)	1 223 256	1 025 434	160 162	37 660	84
vedecká výchova štipendiá (640)	121 762	121 762	0	0	100
poistné a príspevok do poisťovní (620)	423 533	353 488	57 072	12 973	83
tovary a služby (630)	553 513	223 362	266 377	63 774	40
transfery partnerom projektov (640)	61 748	0	61 748	0	0
<b>2. Kapitálové výdavky</b>	<b>29 942</b>	<b>10 100</b>		<b>19 842</b>	<b>34</b>
z toho: obstarávanie kapitálových aktív	29 942	10 100		19 842	34
kapitálové transfery					

### 12.2. Zdroje financovania organizácie

Tabuľka 12b Zdroje financovania organizácie (skutočnosť k 31. 12. 2021 v €)

Typ organizácie (RO,PO)		Z toho kategórie			
Zdroje	Spolu	Kapitálové zdroje	zdroje na mzdy (610)	zdroje na odvody do poisťovní (620)	zdroje na transfery partnerom projektov
<b>1. kapitola SAV (111)</b>	<b>357 856</b>	<b>10 100</b>		<b>4 251</b>	
z toho: VEGA	117 088			923	
MVTS výskumné projekty	54 163	10 100		1 709	
MVTS podpora	4 018				
SASPRO/MOREPRO					
Vydávanie časopisov					
Vedecká výchova (štipendiá)	121 762				
OTAS (630)	60 825			1 619	
<b>2. ŠF EÚ vr. fin. zo ŠR</b>	<b>145 830</b>		<b>46 874</b>	<b>17 468</b>	
<b>3. medzinárodné grantové projekty</b>	<b>28 401</b>	<b>4 500</b>	<b>15 271</b>	<b>5 337</b>	

z toho: H2020	28 401	4 500	15 271	5 337	
<b>4. iné štátne a verejné zdroje (spolu)</b>	<b>394 200</b>		<b>113 287</b>	<b>39 603</b>	<b>61 748</b>
z toho: APVV	394 200		113 287	39 603	61 748
podpora z kapitoly MŠVVaŠ SR (stimuly)					
<b>5. ostatné zdroje</b>	<b>71 133</b>		<b>21 689</b>	<b>7 391</b>	
z toho: príjmy z prenájmu					
príjmy z podnikateľskej činnosti					
príjmy z expertnej činnosti a služieb	71 133		21 689	7 391	

### 13. Nadácie a fondy pri organizácii SAV

### 14. Informácie o aktivitách súvisiacich s uplatňovaním princípov rodovej rovnosti

#### 14.1. Stručné hodnotenie stavu uplatňovania princípov rodovej rovnosti v organizácii, súvisiace aktivity a opatrenia

ÚACH SAV sa prihlásil k dokumentu Plán rodovej rovnosti SAV (Gender Equality Plan, PRR) vypracovaný riešiteľmi projektu ATHENA (Ústav výskumu sociálnej komunikácie SAV). Na ÚACH platia všetky pravidlá odmeňovania a prístupu k informáciám ako aj k možnostiam zastávať vedúce pozície (v kolektívnych orgánoch, v projektoch atd) sú rovnaké pre mužov aj ženy.

#### 14.2. Rodová skladba hlavných riešiteľov (vedúcich) projektov

Tabuľka 14a Rodová skladba hlavných riešiteľov domácich projektov

ŠTRUKTÚRA PROJEKTOV	Organizácia SAV je nositeľom projektu			Organizácia SAV je zmluvným partnerom		
	Počet	Hlavný riešiteľ		Počet	Hlavný riešiteľ za organizáciu	
		Muž	Žena		Muž	Žena
1. Projekty VEGA	10	6	4	3	1	2
2. Projekty APVV	6	3	3	6	3	3
3. Projekty EŠIF	0	0	0	1	1	0
4. Projekty SASPRO, MoRePro	0	0	0	0	0	0
5. Iné projekty (FM EHP, Vedecko-technické projekty, na objednávku rezortov a pod.)	1	1	0	0	0	0

Tabuľka 14b Rodová skladba hlavných riešiteľov medzinárodných projektov

ŠTRUKTÚRA PROJEKTOV	Organizácia SAV je nositeľom projektu			Organizácia SAV je zmluvným partnerom		
	Počet	Hlavný riešiteľ		Počet	Hlavný riešiteľ za organizáciu	
		Muž	Žena		Muž	Žena
<b>1. Projekty Horizont 2020 a Horizont Európa</b>	0	0	0	1	1	0
<b>2. Projekty ERA.NET, ESA, JRP</b>	2	2	0	0	0	0
<b>3. Projekty COST</b>	0	0	0	0	0	0
<b>4. Projekty EUREKA, NATO, UNESCO, CERN, IAEA, IVF, ERDF a iné</b>	0	0	0	1	0	1
<b>5. Projekty v rámci medzivládnych dohôd</b>	0	0	0	0	0	0
<b>6. Bilaterálne projekty MAD, Mobility, Open Mobility</b>	2	2	0	0	0	0
<b>7. Bilaterálne projekty ostatné</b>	2	1	1	1	1	0
<b>8. Podpora MVTS z národných zdrojov okrem SAV (APVV a iné)</b>	1	1	0	0	0	0
<b>9. SAS-UPJŠ ERC Visiting Fellowship Grants</b>	0	0	0	0	0	0
<b>10. Iné projekty</b>	0	0	0	0	0	0

### 14.3. Výskum zameraný na rodovú problematiku

*Uved'te stručné, základné informácie o projektoch orientovaných na rodovú problematiku, ak organizácia takýto výskum realizuje. Informácie o financovaní a výsledkoch takýchto projektov sa nachádzajú v kapitole 2 a v prílohe C.*

## 15. Iné významné činnosti organizácie SAV

V roku 2020 na ústave prebehli rozsiahle rekonštrukčné práce odpadov na budove. Žiaľ, v tejto súvislosti treba upozorniť na nesystematický prístup k plánovaniu prác ale aj k ich vykonávaniu. Podobný problém sprevádzal aj rekonštrukciu rozvodov vody, kedy do dnešného dňa riaditelia dotknutých ústavov nemajú k dispozícii zakreslenie skutočného stavu (teda ani do konca roka 2021). Problémy, ktoré vznikali počas prác boli zo strany kompetentných riešené povrchno, narychlo a bez záujmu, a dokonca možno povedať aj nezodpovedne.

V rámci projektu CEMEA, ktorý sa začal riešiť v priebehu roka 2019 prebehli búracie práce dreveného pavilónu. Na danom mieste je naplánovaná výstavba novej budovy. Momentálne sa stále čaká na vyhodnotenie verejného obstarania zhotoviteľa.

## 16. Vyznamenania, ocenenia a ceny udelené pracovníkom organizácie v roku 2021

### 16.1. Domáce ocenenia

#### 16.1.1. Ocenenia SAV

##### **Boháč Peter**

Čestné uznanie za Súťaž mladých vedeckých pracovníkov SAV

Oceňovateľ: Predsedníctvo SAV

Opis: Prednáška: *Photophysical properties of hybrid systems based on layered silicates and cyanine dyes*, 26.4.2021

##### **Komorovský Stanislav**

Ocenenie predsedníctva Slovenskej akadémie vied, špičková publikácia SAV v kategórii publikácie vo vedeckých časopisoch s najvyšším impaktom podľa SJR

Oceňovateľ: Predsedníctvo SAV

Opis: Autori článku (DOI: 10.1021/acs.chemrev.9b00785) sformulovali nový fundamentálny koncept v NMR spektroskopii čím výrazne posunuli vedecké poznanie NMR spektier chemických zlúčenín obsahujúcich jeden ťažký prvok (ako napríklad irídium, platina, zlato, ortuť, ...). Článok predstavuje štúdiu v ktorej sú vysvetlené nezvyčajné NMR posuny ľahkých prvkov nachádzajúcich sa v blízkosti ťažkého prvku. Vďaka prítomnosti ťažkých elementov museli autori zahrnúť do uvažovania Diracovu relativistickú kvantovú teóriu. Tento pokrok otvára široké možnosti pri výskume látok obsahujúcich ťažké prvky, ako napríklad pri dizajne nových liekov proti rakovine, či pri študovaní šírenia uniknutého jadrového odpadu do prostredia.

##### **Korenko Michal**

Špičková publikácia SAV v kategórii "Publikácie vo vedeckých časopisoch registrovaných v databáze Nature Index"

Oceňovateľ: Predsedníctvo SAV

Opis: Za prácu: Rakhmatullin A.\*, Šimko F.\*, Veron E., Allix M., Martineau-Corcus C., Fitch A., Fayon F., Shakhovoy R., Okhotnikov K., Sarou-Kanian V., Korenko M., Netriová Z. and Bessada C. X-ray diffraction, NMR studies, and DFT calculations of the room and high temperature structures of rubidium cryolite, Rb3AlF6. *Inorganic Chemistry* 59(9), 2020, 6308-6318; Doi: 10.1021/acs.inorgchem.0c00415

##### **Liška Marek**

Medaila za podporu vedy

Oceňovateľ: Predsedníctvo SAV

##### **Madejová Jana**

Zlatá medaila SAV (28. septembra 2021)

Oceňovateľ: Predsedníctvo SAV



Opis: 28. septembra 2021

### **Netriová Zuzana**

Špičková publikácia SAV v kategórii “Publikácie vo vedeckých časopisoch registrovaných v databáze Nature Index”

Oceňovateľ: Predsedníctvo SAV

Opis: Za prácu: Rakhmatullin A.\*, Šimko F.\*, Veron E., Allix M., Martineau-Corcos C., Fitch A., Fayon F., Shakhovoy R., Okhotnikov K., Sarou-Kanian V., Korenko M., Netriová Z. and Bessada C. X-ray diffraction, NMR studies, and DFT calculations of the room and high temperature structures of rubidium cryolite,  $\text{Rb}_3\text{AlF}_6$ . Inorganic Chemistry 59(9), 2020, 6308-6318; Doi: 10.1021/acs.inorgchem.0c00415

### **Šimko František**

Špičková publikácia SAV v kategórii “Publikácie vo vedeckých časopisoch registrovaných v databáze Nature Index”

Oceňovateľ: Predsedníctvo SAV

Opis: Za prácu: Rakhmatullin A.\*, Šimko F.\*, Veron E., Allix M., Martineau-Corcos C., Fitch A., Fayon F., Shakhovoy R., Okhotnikov K., Sarou-Kanian V., Korenko M., Netriová Z. and Bessada C. X-ray diffraction, NMR studies, and DFT calculations of the room and high temperature structures of rubidium cryolite,  $\text{Rb}_3\text{AlF}_6$ . Inorganic Chemistry 59(9), 2020, 6308-6318; Doi: 10.1021/acs.inorgchem.0c00415

## **16.1.2. Iné domáce ocenenia**

## **16.2. Medzinárodné ocenenia**

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

## **18. Problémy a podnety pre činnosť SAV**

Zásadný problém, ktorý narastá niekoľko rokov a v roku 2021 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 organizáciám v tejto situácii je vítaná.

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 schvaľovací proces.

Ďalším problémom presahujúcim možnosti riešenia jednotlivcej organizácie, 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.

Treba spomenúť aj problematiku ohľadne GDPR. Zavedenie tejto smernice komplikuje fungovanie ústavu na všetkých úrovniach od napr. organizovania konferencií, cez používanie výpočtovej techniky, až po napr. zverejňovanie telefónnych čísel na webe. Problémy spojené s touto

problematikou ochromujú v mnohých oblastiach fungovanie vedeckej inštitúcie.

**Správu o činnosti organizácie SAV spracoval(i):**

Zdena Kapišinská,  
doc. Ing. Zoltán Lenčes, PhD., 02/59410408  
Ing. Helena Pálková, PhD., 02/59410485

Schválila vedecká rada organizácie SAV dňa 27.1.2022

**Riaditeľ organizácie SAV**

**Predseda vedeckej rady**

.....  
doc. Ing. Miroslav Boča, DrSc.

.....  
RNDr. Jana Madejová, DrSc.

## Prílohy

### Príloha A

#### Zoznam zamestnancov a doktorandov organizácie k 31.12.2021

##### Zoznam zamestnancov podľa štruktúry

	Meno s titulmi	Úväzok (v %)	Ročný prepočítaný úväzok
<b>Vedúci vedeckí pracovníci DrSc.</b>			
1.	doc. Ing. Miroslav Boča, DrSc.	100	1.00
2.	prof. RNDr. Juraj Bujdák, DrSc.	50	0.50
3.	prof. Ing. Dušan Galusek, DrSc.	55	0.55
4.	prof. Ing. Marek Liška, DrSc., Dr.h.c.	50	0.50
5.	RNDr. Jana Madejová, DrSc.	100	1.00
6.	Dr. Oľga Malkin, DrSc.	100	1.00
7.	Dr. Vladimír Malkin, DrSc.	100	1.00
8.	prof. RNDr. Pavol Šajgalík, DrSc.	55	0.53
<b>Samostatní vedeckí pracovníci</b>			
1.	doc. Ing. Tomáš Bučko, PhD.	25	0.25
2.	Ing. Ondrej Hanzel, PhD.	100	1.00
3.	doc. Ing. Miroslav Hnatko, PhD.	100	1.00
4.	doc. Ing. Mária Chromčíková, PhD.	60	0.86
5.	Mgr. Ľuboš Jankovič, PhD.	100	1.00
6.	Mgr. Stanislav Komorovský, PhD.	100	1.00
7.	Ing. Michal Korenko, PhD.	100	1.00
8.	Ing. Blanka Kubíková, PhD.	100	1.00
9.	doc. Ing. Zoltán Lenčoš, PhD.	100	1.00
10.	Ing. Monika Micháľková, PhD.	75	0.75
11.	Ing. Jarmila Mlynáriková, PhD.	100	1.00
12.	Mgr. Jan Novotný, PhD.	50	0.69
13.	Ing. Helena Páľková, PhD.	100	1.00
14.	Ing. Viliam Pavlík, PhD.	100	1.00
15.	Ing. Anna Prnová, PhD.	100	1.00
16.	Ing. Jaroslav Sedláček, PhD.	100	1.00
17.	Ing. Eva Scholtzová, CSc.	100	1.00
18.	Ing. František Šimko, PhD.	100	1.00
19.	Mgr. Peter Švančárek, PhD.	100	1.00
20.	Ing. Peter Tatarko, PhD.	100	1.00

21.	Mgr. Monika Tatarková, PhD.	100	1.00
22.	Ing. Štefan Varga, CSc.	25	0.25
<b>Vedeckí pracovníci</b>			
1.	James Richard Asher, PhD	100	1.00
2.	Ing. Martin Barlog, PhD.	100	0.33
3.	Mgr. Peter Boháč, PhD.	100	1.00
4.	Mgr. Roman Bystrický, PhD.	20	0.20
5.	doc. RNDr. Edmund Dobročka, CSc.	20	0.20
6.	Ing. Michal Hičák, PhD.	100	0.08
7.	doc. Mgr. Anna Kityk, PhD.	40	0.07
8.	Mgr. Valéria Kureková, PhD.	100	0.00
9.	Mgr. Marián Matejdes, PhD.	33	0.08
10.	Oksana Matselko, PhD.	100	0.83
11.	MSc. Daniel Moreno, PhD.	100	0.33
12.	Ing. Zuzana Netriová, PhD.	125	1.10
13.	Mgr. Marek Pribus, PhD.	100	1.00
14.	RNDr. Veronika Silliková, PhD.	100	1.00
15.	Ing. Michal Slaný, PhD.	100	1.00
16.	Mgr. Tímea Šimonová, PhD.	100	0.66
17.	Ing. Peter Škorňa, PhD.	100	1.00
18.	Ing. Jana Valúchová, PhD.	100	1.00
19.	Ing. Zuzana Vasková, PhD.	100	0.58
<b>Odborní pracovníci s VŠ vzdelaním (výskumní a vývojoví zamestnanci)</b>			
1.	Ing. Martin Barlog, PhD.	28	0.28
2.	Ing. Eva Hadzimová	100	1.00
3.	Ing. Iveta Macková	100	1.00
4.	Dr. Aliasghar Najafzadehkhoe	100	1.00
5.	Ing. Jozef Priščák	100	1.00
6.	MSc. Hakan Ünsal	20	0.20
7.	Mgr. Pavol Weiner	100	1.00
<b>Odborní pracovníci s VŠ vzdelaním (ostatní zamestnanci)</b>			
1.	Ing. Ingrid Hierwegová	5	0.05
2.	Ing. Elena Krippelová	100	1.00
3.	Mgr. Martina Pakanová	100	1.00
4.	Ing. Jaroslav Rusnák, PhD.	33	0.33

5.	JUDr. Bc. Marica Slaná	100	1.00
<b>Odborní pracovníci ÚSV</b>			
1.	Miroslav Baďura	20	0.20
2.	Iveta Bouadjenak	100	1.00
3.	Slavomír Daniš	100	1.00
4.	Miriám Hnatková	100	1.00
5.	Anna Jurová	100	1.00
6.	Zdena Kapišinská	35	0.35
7.	Anna Kovárová	100	1.00
8.	Mária Strempeková	100	1.00
9.	Alexandra Tonkovičová	100	1.00
10.	Denisa Žilinská	100	0.16
<b>Ostatní pracovníci</b>			
1.	Anna Jurová	20	0.20
2.	Ingrida Kutašovičová	100	1.00
3.	Ing. Iveta Macková	20	0.20
4.	Terézia Pírová	100	1.00

**Zoznam zamestnancov, ktorí odišli v priebehu roka**

	Meno s titulmi	Dátum odchodu	Ročný prepočítaný úväzok
<b>Odborní pracovníci s VŠ vzdelaním (výskumní a vývojoví zamestnanci)</b>			
1.	Ing. Martin Barlog, PhD.	31.12.2021	0.28
2.	Ing. Michal Hičák	30.11.2021	0.55
3.	Ing. Eva Mikšíková	31.8.2021	0.83
<b>Odborní pracovníci s VŠ vzdelaním (ostatní zamestnanci)</b>			
1.	Ing. Rastislav Haška	31.5.2021	0.42
<b>Odborní pracovníci ÚSV</b>			
1.	Alexandra Dominika Drahošová	30.11.2021	0.97
2.	Jarmila Heinleinová	31.5.2021	0.41

**Zoznam doktorandov**

	Meno s titulmi	Škola/fakulta	Študijný odbor
<b>Interní doktorandi hrazení z prostředkov SAV</b>			
1.	MSc. Ramu Ambati	Prírodovedecká fakulta UK	
2.	MSc. Sanam Bashir	Prírodovedecká fakulta UK	

3.	Guido Manuel De La Torre Olvera	Prírodovedecká fakulta UK	
4.	MSc. Alper Guneren	Prírodovedecká fakulta UK	
5.	Naser Hosseini	Prírodovedecká fakulta UK	
6.	MSc. Dhiya Krishnan	Prírodovedecká fakulta UK	
7.	Florian Andreas Lemken	Prírodovedecká fakulta UK	
8.	Mgr. Jakub Michalík	Fakulta chemickej a potravinárskej technológie STU	
9.	Mgr. Debora Mišenková	Prírodovedecká fakulta UK	
10.	Mgr. Patrícia Petrisková	Prírodovedecká fakulta UK	4.1.15 anorganická chémia
11.	Eva Skoura	Prírodovedecká fakulta UK	
12.	MSc. Hakan Ünsal	Prírodovedecká fakulta UK	4.1.15 anorganická chémia
13.	Inga Zhukova	Prírodovedecká fakulta UK	
<b>Interní doktorandi hrazení z iných zdrojov</b>			
<i>organizácia nemá interných doktorandov hrazených z iných zdrojov</i>			
<b>Externí doktorandi</b>			
<i>organizácia nemá externých doktorandov</i>			

**Zoznam zamestnancov prijatých do jedného roka od získania PhD.**

	Meno s titulmi	Dátum obhajoby	Dátum prijatia	Úväzok (v %)
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**Zoznam emeritných vedeckých zamestnancov**

	Meno s titulmi
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**Príloha B****Projekty riešené v organizácii****Medzinárodné projekty****Programy: Medziakademická dohoda (MAD)****1.) Vývoj nových pokročilých keramických kompozitov pre vesmírne aplikácie** (*Development of new advanced ceramic composites for aerospace industry*)

<b>Zodpovedný riešiteľ:</b>	Peter Tatarko
<b>Trvanie projektu:</b>	1.1.2018 / 31.12.2021
<b>Evidenčné číslo projektu:</b>	2/0116/17
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	1 - Česko: 1
<b>Čerpané financie:</b>	-

**Dosiahnuté výsledky:**

V poslednom roku riešenia projektu boli vedecké aktivity zamerané na prípravu a štúdium vlastností materiálov na báze ZrB<sub>2</sub>-SiC s rôznym obsahom Yb<sub>2</sub>O<sub>3</sub> (2, 5 a 10 hmot.%), pričom materiály boli pripravené dvoma rôznymi spôsobmi, t.j. reakčným a konvenčným spekaním. Pomocou reakčného spekania bolo možné pripraviť plne hutné materiály identického zloženia pri teplote o 400°C nižšej ako v prípade konvenčného spekania (2000°C vs. 1600°C). Počas reakčného spekania sa tvoria fázy SiC a ZrB<sub>2</sub> in-situ reakciou medzi B<sub>4</sub>C, ZrSi<sub>2</sub> a C, čo vedie k jemnozrnejšej mikroštruktúre materiálov. Za najdôležitejší výsledok možno považovať skutočnosť, že použitím metódy reakčného spekania došlo k výraznému zníženiu teploty zhutnenia vysokoteplotných keramických materiálov, pričom výrazne jemnozrnejšia mikroštruktúra bola príčinou vyššej tvrdosti a odolnosti materiálov proti ablácií pri extrémne vysokých teplotách (do 2700°C) v porovnaní s konvenčne pripravenými materiálmi. Príprava materiálov, ako aj skúšky odolnosti proti ablácií boli realizované na ÚACH, pričom mechanické vlastnosti boli študované na partnerskom pracovisku Ústavu fyziky materiálu AVČR v Brne.

Okrem toho, bola spolupráca orientovaná na hodnotenie mechanických vlastností konštrukčnej keramiky na báze SiC, B<sub>4</sub>C a Si<sub>3</sub>N<sub>4</sub> zhutnenej pomocou grafénových nanodoštičiek a nanodoštičiek nitridu bóru.

**Výstupy:**

1. HANZEL, Ondrej\*\* - LENČEŠ, Zoltán - TATARKO, Peter - SEDLÁK, Richard - DLOUHÝ, Ivo - DUSZA, Ján - ŠAJGALÍK, Pavol. Preparation and properties of layered SiC-graphene composites for EDM. In Materials, 2021, vol. 14, no. 11, p. 2916-1-2916-14. (2020: 3.623 - IF, Q1 - JCR, 0.682 - SJR, Q2 - SJR). ISSN 1996-1944. Dostupné na: <https://doi.org/10.3390/ma14112916>
2. ÜNSAL, Hakan - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - TATARKOVÁ, Monika - DLOUHÝ, Ivo - TATARKO, Peter\*\*. In-situ graphene platelets formation and its suppression during reactive spark plasma sintering of boron carbide/titanium diboride composites. In Journal of the European Ceramic Society, 2021, vol. 41, no. 13, p. 6281-6289. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.06.053>
3. TATARKOVÁ, Monika\*\* - TATARKO, Peter - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - DUSZA, Ján - ŠAJGALÍK, Pavol. Influence of hexagonal boron nitride nanosheets on phase transformation, microstructure evolution and mechanical properties of Si<sub>3</sub>N<sub>4</sub> ceramics. In Journal of the European Ceramic Society, 2021, vol. 41, no. 10, p. 5115-5126. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.01.057>
4. ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - MATOVIC, Branko - TATARKOVÁ, Monika - CHLUP, Zdeněk - HIČÁK, Michal - DLOUHÝ, Ivo - TATARKO, Peter. In situ synthesis and characterization of ZrB<sub>2</sub>-SiC ceramics with rare-earth based additives. In CYSC-2021. 14th ECerS Conference for Young Scientists in Ceramics, October 20-23, 2021, Novi Sad, Serbia : Book of Abstracts. - Novi Sad, Serbia : Faculty of Technology, University of Novi Sad, Serbia, 2021, p. 43-44. ISBN 978-86-6253-136-0. (CYSC-2021. ECerS Conference for Young Scientists in Ceramics)



**Programy: Multilaterálne - iné****2.) Atómová koncepcia materiálov na báze uhlíka pre novú normálnu spoločnosť** (*Atomic Design of Carbon-Based Materials for New Normal Society*)

<b>Zodpovedný riešiteľ:</b>	Eva Scholtzová
<b>Trvanie projektu:</b>	1.11.2021 / 30.10.2024
<b>Evidenčné číslo projektu:</b>	V4-Japan Joint Research Program
<b>Organizácia je koordinátorom projektu:</b>	nie
<b>Koordinátor:</b>	Advanced Institute for Materials Research (AIMR) Tohoku University Sendai
<b>Počet spoluriešiteľských inštitúcií:</b>	5 - Kanada: 1, Česko: 1, Maďarsko: 1, Japonsko: 1, Poľsko: 1
<b>Čerpané financie:</b>	SAV: 4167 €

**Dosiahnuté výsledky:**

Projekt začal 1.11.2021 a hlavnou úlohou Slovenskej strany v tomto projekte je modelovanie štruktúr materiálov na báze uhlíka (MBU) a štúdium ich vlastností rozličnými výpočtovými metódami na rôznom stupni teórie. Na atomárnej úrovni sa na sérii klastrových a periodických modelov s obsahom pyrolického dusíka s rôznymi možnými produktami disociácie začali študovať disociačné procesy pri teplotne programovanej desorpcii (TPD) MBU, konkrétne N dopovaného grafénu ab initio DFT metódou. Predbežné výsledky ukazujú, že disociáciou C-N väzby vzniká CNH produkt a energeticky výhodnejší HCN product disociáciou C-C väzby. Boli pozorované rovnaké trendy pre malé klastrové a veľké periodické modely. Ďalej boli pripravené periodické štruktúrne modely grafénu a modifikovaného defektného grafénu (prítomné 5 a 7 členné kruhy ako defekty) a použité na výpočet Ramanovského spektra. Typický D pás, charakteristický pre prítomnosť defektov v graféne, bol detegovaný pri 1385 cm<sup>-1</sup>, čo je v dobrej zhode s experimentálnou hodnotou 1338 cm<sup>-1</sup> nameranou pre GMS materiál pripravený japonskými partnermi. Okrem toho sa analyzovalo aj prerozdelenie elektrónovej hustoty v dôsledku prítomných defektov. Výsledky budú prezentované na Kick-off online mítingu AtomDeC projektu 18.1. - 19.1.2022 formou prednášky a posteru.

**Programy: Bilaterálne - iné****3.) Heat Capacities of fluorozirconate compounds** (*Heat Capacities of fluorozirconate compounds*)

<b>Zodpovedný riešiteľ:</b>	Miroslav Boča
<b>Trvanie projektu:</b>	1.1.2021 / 31.12.2021
<b>Evidenčné číslo projektu:</b>	SFERA3; SURPF2001310039
<b>Organizácia je koordinátorom projektu:</b>	nie
<b>Koordinátor:</b>	ENEA - Casaccia Research Center Taliansko
<b>Počet spoluriešiteľských inštitúcií:</b>	0
<b>Čerpané financie:</b>	-

**Dosiahnuté výsledky:**

V rámci riešenia projektu boli detailne študované tepelné kapacity troch rozdielnych fluorozirkóniových zlúčenín, ktoré sa líšili prítomnými fázovými prechodmi v tuhom stave i teplotou topenia. Výsledky ukázali, že hodnoty tepelných kapacít v študovanom teplotnom intervale sa výrazne nelíčili a dosahovali hodnoty okolo 1J g<sup>-1</sup> °C<sup>-1</sup>. Výraznejšie zmeny v hodnotách tepelných kapacít fluorozirkóniových zlúčenín neboli pozorované ani po pridaní nanočastíc Al<sub>2</sub>O<sub>3</sub>.

**4.) Percepcia spinovej interakcie na pokročilej úrovni** (*Spin Coupling Advanced Level Perception*)

<b>Zodpovedný riešiteľ:</b>	Oľga Malkin
<b>Trvanie projektu:</b>	1.2.2020 / 31.12.2022
<b>Evidenčné číslo projektu:</b>	SK-FR-19-0001
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	1 - Francúzsko: 1
<b>Čerpané financie:</b>	-

Dosiahnuté výsledky:

Boli vyvinuté prístupy na analýzu viacerých spin-spinových väzobných dráh v komplexných systémoch vrátane komplexov prechodných kovov a aplikované na niekoľko systémov. Zodpovedajúci rukopis je v záverečnej fáze prípravy.

### 5.) Vysokoteplotné karbidy pre aplikácie v extrémnych podmienkach (*Ultra-high temperature carbides for extreme environment applications*)

<b>Zodpovedný riešiteľ:</b>	Peter Tatarko
<b>Trvanie projektu:</b>	1.1.2019 / 31.12.2021
<b>Evidenčné číslo projektu:</b>	SK-SRB-18-0022
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	1 - Srbsko: 1
<b>Čerpané financie:</b>	-
	Podpora medzinárodnej spolupráce z národných zdrojov:
	1823 €

Dosiahnuté výsledky:

Riešenie projektu bolo zamerané na porovnanie mikroštruktúry a mechanických vlastností kompozitných B<sub>4</sub>C-TiB<sub>2</sub> materiálov, pripravených 3 rôznymi spôsobmi (reakčný spark plasma sintering, konvenčný spark plasma sintering, a konvenčné žiarové lisovanie). Bolo jednoznačne preukázané, že najviac homogénna a jemnozrnná mikroštruktúra, ako aj najlepšia kombinácia mechanických vlastností bola dosiahnutá použitím reakčného spekania. Ďalšou aktivitou v rámci tejto medzinárodnej spolupráce bola tiež teoretická predikcia štruktúry a vlastností materiálu SiB<sub>6</sub> pre extrémne aplikácie. Spolupráca bola orientovaná aj na štúdium mechanických vlastností kompozitných ZrB<sub>2</sub>-SiC materiálov s prídavkom pyrochlórnej fázy Yb<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>. Táto fáza bola pripravená na srbskom pracovisku, pričom finálne kompozity boli pripravené na ÚACH SAV. Za najdôležitejší výsledok možno považovať skutočnosť, že prídavok 10 hmot.% pyrochlórnej fázy viedol k trojnásobne lepšej odolnosti proti ablácii, pričom mechanické vlastnosti pri izbovej teplote ostali porovnateľné s vlastnosťami materiálu ZrB<sub>2</sub>-SiC bez pyrochlórnej fázy.

## Výstupy:

1. ÜNSAL, Hakan - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - TATARKOVÁ, Monika - DLOUHÝ, Ivo - TATARKO, Peter\*\*. In-situ graphene platelets formation and its suppression during reactive spark plasma sintering of boron carbide/titanium diboride composites. In Journal of the European Ceramic Society, 2021, vol. 41, no. 13, p. 6281-6289. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Typ: ADCA. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.06.053>
2. ŠKUNDRIĆ, Tamara - MATOVIC, Branko - ZARUBICA, Aleksandra - ZAGORAC, Jelena - TATARKO, Peter - ZAGORAC, Dejan\*\*. Structure prediction and mechanical properties of silicon hexaboride on ab initio level. In Materials, 2021, vol. 14, p. 7887-1-7887-17. (2020: 3.623 - IF, Q1 - JCR, 0.682 - SJR, Q2 - SJR, karentované - CCC). Typ: ADCA. Dostupné na: <https://doi.org/10.3390/ma14247887>
3. ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - MATOVIC, Branko - TATARKOVÁ, Monika - CHLUP, Zdeněk - HIČÁK, Michal - DLOUHÝ, Ivo - TATARKO, Peter. In situ synthesis and characterization of ZrB<sub>2</sub>-SiC ceramics with rare-earth based additives. In CYSC-2021. 14th ECerS Conference for Young Scientists in Ceramics, October 20-23, 2021, Novi Sad, Serbia : Book of Abstracts. - Novi Sad, Serbia : Faculty of Technology, University of Novi Sad, Serbia, 2021, p. 43-44. ISBN 978-86-6253-136-0. (CYSC-2021. ECerS Conference for Young Scientists in Ceramics). Typ: AFG
4. TATARKO, Peter - MATOVIC, Branko - GRASSO, Salvatore - ZHOU, Xiaobing - DLOUHÝ, Ivo - REECE, Michael J. - FERRARIS, Monica. Joining and integration of silicon carbide based ceramics. In CYSC-2021. 14th ECerS Conference for Young Scientists in Ceramics, October 20-23, 2021, Novi Sad, Serbia : Book of Abstracts. Eds. in Chief Vladimir V. Srdić, Andraž Kocjan, Maria Canillas Perez. - Novi Sad, Serbia : Faculty of Technology, University of Novi Sad, Serbia, 2021, p. 19-20. ISBN 978-86-6253-136-0. (CYSC-2021. ECerS Conference for Young Scientists in Ceramics). Typ: AFE

## Programy: Horizont 2020

### 6.) Sodium-Ion and sodium Metal Batteries for efficient and sustainable next-generation energy storage (*Sodium-Ion and sodium Metal Batteries for efficient and sustainable next-generation energy storage*)

<b>Zodpovedný riešiteľ:</b>	Zoltán Lenčes
<b>Trvanie projektu:</b>	1.1.2021 / 31.12.2024
<b>Evidenčné číslo projektu:</b>	963542
<b>Organizácia je koordinátorom projektu:</b>	nie
<b>Koordinátor:</b>	Technische Universität Darmstadt
<b>Počet spoluriešiteľských inštitúcií:</b>	14 - Nemecko: 2, Francúzsko: 3, Veľká Británia: 3, Holandsko: 1, Nórsko: 2, Švédsko: 2, Ukrajina: 1
<b>Čerpané financie:</b>	SAV: 4018 € EU: 28401 €

#### Dosiahnuté výsledky:

Vysokoporézne keramické anódy pre sodíkové batérie boli pripravené z pyrolyzovaného Si-O-C polymérneho prekursoru Polyramic, resp. zo zmesi práškov pyrolyzovaného polyméru, kremíka a uhlíka. Boli optimalizované podmienky zosieťovania polyméru (250 °C/3 h) a následnej pyrolýzy pri 900 °C/3 h a 1200 °C/1 h v atmosfére argónu alebo dusíka. Prvotné experimenty ukázali, že veľkosť častíc Si a C prášku má vplyv na vlastnosti batérií, z toho dôvodu boli optimalizované podmienky mletia práškov. Bolo vykonaných 20 mlecích experimentov s rôznymi podmienkami mletia a na základe získaných výsledkov boli vytvorené regresné rovnice na odhad vstupných parametrov mletia (rýchlosť otáčania planetového mlynu, čas mletia, pomer prášok/etanol, pomer prášok/mlecie guľičky) na výsledné vlastnosti mletého prášku (úroveň kontaminácie prášku, veľkosť kryštalitov a veľkosť častíc. Pomocou modelových výpočtov boli stanovené podmienky mletia (rýchlosť mletia 320 rpm, čas 12 hod, pomer etanol/prášok = 5, pomer guľičky/prášok = 9,5) aby bola úroveň kontaminácie nižšia ako 1%, veľkosť kryštalitov pod 40 nm, veľkosť častíc D10 < 1,5 µm, D90 < 8,1 µm. Analýza mletých práškov ukázala, že modelové výpočty podmienok mletia vykazujú 95% spoľahlivosť. Z mletých práškov boli pripravené stabilné suspenzie na základe reologických meraní a odliate tenké vrstvy keramických anód. V glove-boxe boli zhotovené batérie, pričom boli použité komerčné elektrolyty a katódy. Galvanostatické nabíjacie-vybíjacie testy boli uskutočnené pri rôznych prúdových hustotách (0,2 – 4,0 A·g<sup>-1</sup>). Výsledky meraní ukázali že po prvých 3-5 cykloch nabíjania – vybíjania dochádza k prudkému poklesu špecifickej kapacity z 1000 mAh/g na 400 mAh/g. V ostatných cykloch (max. 100 cyklov) dochádzalo k miernemu poklesu kapacity zo 400 mAh/g na cca 200 mAh/g.

## Programy: JRP

### 7.) Štruktúry a biokompozity pre regeneráciu tkanív (*Scaffolds and biocomposites for tissue regeneration*)

<b>Zodpovedný riešiteľ:</b>	Dušan Galusek
<b>Trvanie projektu:</b>	1.1.2019 / 31.12.2021
<b>Evidenčné číslo projektu:</b>	SAS-MOST JRP 2018/02
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	2 - Taiwan: 2
<b>Čerpané financie:</b>	SAV: 24996 €

#### Dosiahnuté výsledky:

V treťom roku riešenia projektu boli pripravené mezoporézne bioaktívne sklené nanočastice (MBGNP) dopované Ce a Ga mikroemulznou metódou sol-gél v binárnom systéme SiO<sub>2</sub>-CaO. Všetky MBGNP, s výnimkou nanočastíc dopovaných viac ako 1 mol % Ce boli in bioaktívne in vitro, vykazovali antibakteriálnu aktivitu proti *S. aureus* a *E. coli* bez cytotoxického efektu voči osteoblastovým bunkám MG-63. Skúmal sa tiež účinok vplyv parametrov syntézy (najmä pomeru HCl/H<sub>3</sub>PO<sub>4</sub>) pri príprave mezoporéznych nanotyčínok oxidu kremičitého (SBA-15). Kombinácia zmesi kyslík so silánovým prekursorom modifikovaným glycerolom umožnila prípravu bioaktívnych mezoporéznych nanotyčínok s vyššou degradovateľnosťou a nízkou cytotoxicitou voči osteoblastom MC3T3-E1.

1. KURTULDU, Fatih - MUTLU, Nurshen - MICHÁLEK, Martin - ZHENG, Kai - MASAR, Milan - LIVERANI, Liliana - CHEN, Si - GALUSEK, Dušan - BOCCACCINI, Aldo. Cerium and gallium containing mesoporous

bioactive glass nanoparticles for bone regeneration: Bioactivity, biocompatibility and antibacterial activity. Mater Sci Eng C. 2021;124. doi:10.1016/j.msec.2021.112050, ADM, Q1

2. ARGAS-OSORIO, Zulema\*\* - KLOTSCHAN, Artem\* - ARANGO-OSPINA, Marcela\* - PINEIRO, Yolanda - LIVERANI, Liliana - RIVAS, José - MICHÁLEK, Martin - GALUSEK, Dušan - BOCCACCINI, Aldo\*\*. Effect of glycerol and H<sub>3</sub>PO<sub>4</sub> on the bioactivity and degradability of rod-like SBA-15 particles with active surface for bone tissue engineering applications. In Microporous and Mesoporous Materials, 2022, vol. 329, p. 111543-1-111543-12. Dostupné na: <https://doi.org/10.1016/j.micromeso.2021.111543> Typ: ADCA

## 8.) Vývoj bioaktívneho funkčne gradientného nitridu kremičitého (*Development of functionally graded silicon nitride with improved bioactivity*)

<b>Zodpovedný riešiteľ:</b>	Miroslav Hnatko
<b>Trvanie projektu:</b>	1.1.2021 / 31.12.2023
<b>Evidenčné číslo projektu:</b>	JRP SAV – TUBITAK 546676
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	1 - Turecko: 1
<b>Čerpané financie:</b>	SAV: 25000 €

### Dosiahnuté výsledky:

Prvý rok riešenia projektu bol zameraný na prípravu pások na báze Si<sub>3</sub>N<sub>4</sub> s rôznym pomerom prísad CaSiO<sub>3</sub> a Y<sub>2</sub>O<sub>3</sub>, ako aj rôznym obsahom pórotvorného činidla. Tieto pásy simulujú jednotlivé „oblasti“ funkčne gradientného materiálu, t.j. hutnú, prechodovú a pórovitú vrstvu. Realizovala sa podrobná štúdia optimalizácie režimu spekania jednotlivých materiálových zložení metódou spekania za asistencie elektrického prúdu (Field Assisted Sintering Technology – FAST) v teplotnom intervale 1600°C – 1750°C. Dôraz sa kládol na pochopenie vplyvu teploty spekania a celkového režimu spekania na transformáciu zŕn nitridu kremičitého, ako aj vplyvu rôzneho pomeru prísad na tvorbu finálnej mikroštruktúry a fázovú transformáciu Si<sub>3</sub>N<sub>4</sub>. Jednotlivé „oblasti“ funkčne gradientného materiálu boli pripravené vo forme pások pozostávajúcich z 12 vrstiev. Tie budú v ďalšom kroku spájané a zhutnené do jedného materiálu.

### Výstupy:

TATARKOVÁ, Monika\*\* - TATARKO, Peter - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - DUSZA, Ján - ŠAJGALÍK, Pavol. Influence of hexagonal boron nitride nanosheets on phase transformation, microstructure evolution and mechanical properties of Si<sub>3</sub>N<sub>4</sub> ceramics. In Journal of the European Ceramic Society, 2021, vol. 41, no. 10, p. 5115-5126. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Typ: ADCA. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.01.057>

## Programy: Mobility

### 9.) Reakčné spájanie pokročilých keramických materiálov na báze SiC (*Reaction bonding of advanced SiC-based ceramics*)

<b>Zodpovedný riešiteľ:</b>	Peter Tatarko
<b>Trvanie projektu:</b>	1.1.2021 / 31.12.2022
<b>Evidenčné číslo projektu:</b>	SAV-AVČR-21-04
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	1 - Česko: 1
<b>Čerpané financie:</b>	SAV: 1000 €

### Dosiahnuté výsledky:

V súlade s plánom pre prvý rok riešenia projektu boli výskumné aktivity zamerané na prípravu vstupných materiálov (CVD-SiC, Cf/SiC, a ZrSi<sub>2</sub>). Za účelom určenia vhodných parametrov pre spájanie, bola realizovaná štúdia zmáčavosti roztavenej zliatiny ZrSi<sub>2</sub> na povrchov CVD-SiC a Cf/SiC. Študoval sa vplyv teploty, výdrže, ale hlavne atmosféry. Výsledky jasne preukázali, že roztavená zliatina ZrSi<sub>2</sub> lepšie zmáča povrch SiC v argónovej atmosfére, nakoľko dochádzalo k výrazným stratám Si pri vysokých teplotách vo vákuu. Na základe výsledkov boli určené najvhodnejšie parametre pre spájanie, a to teplota 1650°C, a argónová atmosféra. Uskutočnili sa prvé pokusy spájania, avšak proces spájania bude ešte optimalizovaný pri ďalšom riešení projektu.

Okrem toho, bola spolupráca orientovaná na hodnotenie mechanických vlastností konštrukčnej keramiky na báze SiC, B<sub>4</sub>C a Si<sub>3</sub>N<sub>4</sub> zhúževnatej pomocou grafénových nanodoštičiek a nanodoštičiek nitridu bóru.

#### Výstupy:

1. HANZEL, Ondrej\*\* - LENČEŠ, Zoltán - TATARKO, Peter - SEDLÁK, Richard - DLOUHÝ, Ivo - DUSZA, Ján - ŠAJGALÍK, Pavol. Preparation and properties of layered SiC-graphene composites for EDM. In Materials, 2021, vol. 14, no. 11, p. 2916-1-2916-14. (2020: 3.623 - IF, Q1 - JCR, 0.682 - SJR, Q2 - SJR). ISSN 1996-1944. Typ: ADCA. Dostupné na: <https://doi.org/10.3390/ma14112916>
2. ÜNSAL, Hakan - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - TATARKOVÁ, Monika - DLOUHÝ, Ivo - TATARKO, Peter\*\*. In-situ graphene platelets formation and its suppression during reactive spark plasma sintering of boron carbide/titanium diboride composites. In Journal of the European Ceramic Society, 2021, vol. 41, no. 13, p. 6281-6289. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Typ: ADCA. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.06.053>
3. TATARKOVÁ, Monika\*\* - TATARKO, Peter - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - DUSZA, Ján - ŠAJGALÍK, Pavol. Influence of hexagonal boron nitride nanosheets on phase transformation, microstructure evolution and mechanical properties of Si<sub>3</sub>N<sub>4</sub> ceramics. In Journal of the European Ceramic Society, 2021, vol. 41, no. 10, p. 5115-5126. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Typ: ADCA. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.01.057>
4. ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - MATOVIC, Branko - TATARKOVÁ, Monika - CHLUP, Zdeněk - HIČÁK, Michal - DLOUHÝ, Ivo - TATARKO, Peter. In situ synthesis and characterization of ZrB<sub>2</sub>-SiC ceramics with rare-earth based additives. In CYSC-2021. 14th ECerS Conference for Young Scientists in Ceramics, October 20-23, 2021, Novi Sad, Serbia : Book of Abstracts. - Novi Sad, Serbia : Faculty of Technology, University of Novi Sad, Serbia, 2021, p. 43-44. ISBN 978-86-6253-136-0. (CYSC-2021. ECerS Conference for Young Scientists in Ceramics). Typ: AFG

## Domáce projekty

### Programy: VEGA

#### 1.) Fázové premeny oxidov kovov v roztavených fluoridových systémoch (*Phase changes of metal oxides in fluoride melts*)

<b>Zodpovedný riešiteľ:</b>	Miroslav Boča
<b>Trvanie projektu:</b>	1.1.2020 / 31.12.2023
<b>Evidenčné číslo projektu:</b>	2/0024/20
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	0
<b>Čerpané financie:</b>	SAV: 21159 €

#### Dosiahnuté výsledky:

V rámci projektu bola študovaná rozpustnosť oxidu lantanitého v dvoch roztavených systémoch: LiF-NaF a LiF-NaF-LaF<sub>3</sub>. Predchádzajúce výsledky ukázali, že rozpustnosť La<sub>2</sub>O<sub>3</sub> v eutektickej zmesi LiF-NaF je nízka. Tieto výsledky boli potvrdené aj v prípade experimentov termickej analýzy s 3-hodinovou výdržou, kde neboli pozorované takmer žiadne rozdiely v teplotách primárnej kryštalizácie, či v eutektickej teplote. Pre získanie ďalších údajov o rozpustnosti oxidu La<sub>2</sub>O<sub>3</sub>, bol pripadávaný do fluoridovej zmesi s obsahom fluoridu lantanitého, pre zvýšenie rozpustnosti oxidu. Prvé experimenty naznačujú, že rozpustnosť by v takýchto roztavených sústavách mohla byť vyššia.

#### 2.) Hlinitano-kremičitanové sklené a sklokeramické materiály spevnené iónovou výmenou a dodatočnými funkčnosťami (*Ion exchange strengthened aluminosilicate glass/glass-ceramics with additional functionalities*)

<b>Zodpovedný riešiteľ:</b>	Dušan Galusek
<b>Trvanie projektu:</b>	1.1.2021 / 31.12.2024
<b>Evidenčné číslo projektu:</b>	VEGA 2/0028/21
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	1 - Slovensko: 1

**Čerpané financie:**

SAV: 7049 €

Dosiahnuté výsledky:**3.) Nové anorganické fosfory na báze stechiometrických hlinitanov a kremičitanov s dlhodobou svetelnou emisiou pre optické a biomedicínske aplikácie** (*Long persistent phosphors on the base of stoichiometric aluminates and silicates for optical and biomedical applications*)**Zodpovedný riešiteľ:**

Dušan Galusek

**Trvanie projektu:**

1.1.2018 / 31.12.2021

**Evidenčné číslo projektu:**

1/0527/18

**Organizácia je koordinátorom projektu:**

nie

**Koordinátor:**

Trenčianska univerzita Alexandra Dubčeka v Trenčíne

**Počet spoluriešiteľských inštitúcií:**

0

**Čerpané financie:**

VEGA MŠ: 4054 €

Dosiahnuté výsledky:

Optimalizovala sa príprava lumínoforov na báze granátových štruktúr  $Gd_3Sc_2Ga_3O_{12}$  a  $La_3Sc_2Ga_3O_{12}$  dopovaných  $Cr^{3+}$  a  $Mn^{4+}$  iónmi reakciou v tuhej fáze. Pripravené lumínofory vykazujú emisiu v červenej spektrálnej oblasti s relatívne dlhou dobou dosvitu. Detailne preštudované boli aj transparentné materiály na báze oxyfluoridových skiel s nanokryštalickou fluoridovou fázou dopované luminiscenčnými aktivátormi v kombinácii  $Er^{3+}, Yb^{3+}$  pre optickú termometriu, teplotné senzory, vhodné aj pre využitie v bio-aplikáciách. Okrem prístupu tepelne spriahnutých energetických hladín v  $Er^{3+}$  pri výpočte parametrov teplotnej citlivosti materiálu, aplikovaná bola aj nová stratégia založená na teplotne nespriahnutých stavoch v  $Er^{3+}$ .

## Výstupy:

1. GRIEBENOW, Kristin\*\* - MUNOZ, Francisco - TAGIARA, Nagia S. - KLEMENT, Róbert - PRNOVÁ, Anna - WOLFRUM, Bruno - KAMITSOS, Efstratios I. - DURAN, Alicia - GALUSEK, Dušan. Structure and fluorescence properties of Dy-doped alkaline-earth borophosphate glasses. In International Journal of Applied Glass Science, 2021, vol. 12, no. 4, p. 472-484. (2020: 2.029 - IF, Q2) Typ: ADCA
2. DAGUPATI, Rajesh\*\* - KLEMENT, Róbert\*\* - GALUSEK, Dušan.  $Er^{3+}/Yb^{3+}$  co-doped oxyfluoro tellurite glasses: Analysis of optical temperature sensing based on up-conversion luminescence. In International Journal of Applied Glass Science, 2021, vol. 12, no. 4, p. 462-471. (2020: 2.029 - IF, Q2)
3. DAGUPATI, Rajesh\*\* - KLEMENT, Róbert\*\*, RAJAVARAM, R - VELÁZQUEZ, José Joaquín - GALUSEK, Dušan, In situ synthesis of beta- $Na_{1.5}Y_{1.5}F_6:Er^{3+}$  crystals in oxyfluoride silicate glass for temperature sensors and their spectral conversion and optical thermometry analysis, Molecules, 26 (2021), 6901.

**4.) Elektromagnetické tienenie funkčne gradientných vrstevnatých kompozitov na báze SiC s prídavkom grafénu a uhlíkových nanorúrok** (*Electromagnetic shielding properties of functionally graded layered SiC-graphene and SiC-carbon nanotubes composites*)**Zodpovedný riešiteľ:**

Ondrej Hanzel

**Trvanie projektu:**

1.1.2021 / 31.12.2024

**Evidenčné číslo projektu:**

2/0007/21

**Organizácia je koordinátorom projektu:**

áno

**Koordinátor:**

Ústav anorganickej chémie SAV

**Počet spoluriešiteľských inštitúcií:**

0

**Čerpané financie:**

SAV: 8403 €

Dosiahnuté výsledky:

V rámci riešenia projektu boli pripravené stabilné keramické suspenzie s rôznym prídavkom grafénových nanoplatničiek (GNPs) a uhlíkových nanorúrok (CNTs). Bol optimalizovaný zeta potenciál daných suspenzií s cieľom zabrániť aglomerácií a sedimentácií uhlíkových nanoštruktúr počas prípravy. Taktiež bola optimalizovaná viskozita daných suspenzií s cieľom pripraviť granulované kompozitné prášky pomocou metódy vymrazovacej granulácie. Následne boli z niektorých kompozitných práškov postupným zalisovaním do formy vytvorené vrstevnaté materiály s usporiadaním vrstiev 0-5-15 % GNPs a vrstevnaté materiály s usporiadaním vrstiev 15-5-0-5-15 % GNPs, ktoré boli spekané metódou rapid hot press (RHP) pri teplote  $1800^{\circ}C$ , vo vákuu po dobu 5 minút a pri tlaku 50 MPa. Relatívna hustota pripravených

3- a 5-vrstvových kompozitov bola vyššia ako 98,7 %.

Na takto pripravených hutných materiáloch bola vykonaná mikroštruktúrna analýza a boli merané funkčné vlastnosti (konkrétne elektrická vodivosť a tepelná difuzivita) v kolmom smere vzhľadom na usporiadanie grafénových platničiek a usporiadanie jednotlivých vrstiev. Elektrická vodivosť 3-vrstvových kompozitných materiálov dosahovala 1442 S/m v prípade merania na strane vrstvy s 15 hm. % GNP, v prípade merania na strane vrstvy SiC bez prídavku grafénu elektrická vodivosť dosahovala 122 S/m. Elektrická vodivosť 5-vrstvových kompozitných materiálov dosahovala 867 S/m z oboch strán. Tieto výsledky dokazujú, že použitie metód vymrazovacej granulácie a spekania v rapid hot presse umožňuje získať hutné vrstevnaté kompozitné materiály SiC-grafén s vysokou elektrickou vodivosťou.

Publikácie:

1. HANZEL, Ondrej\*\* - LENČEŠ, Zoltán - TATARKO, Peter - SEDLÁK, Richard - DLOUHÝ, Ivo - DUSZA, Ján - ŠAJGALÍK, Pavol. Preparation and properties of layered SiC-graphene composites for EDM. In Materials, 2021, vol. 14, no. 11, p. 2916-1-2916-14. (2020: 3.623 - IF, Q1 - JCR, 0.682 - SJR, Q2 - SJR). ISSN 1996-1944. Dostupné na: <https://doi.org/10.3390/ma14112916>.
2. ÜNSAL, Hakan - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - TATARKOVÁ, Monika - DLOUHÝ, Ivo - TATARKO, Peter\*\*. In-situ graphene platelets formation and its suppression during reactive spark plasma sintering of boron carbide/titanium diboride composites. In Journal of the European Ceramic Society, 2021, vol. 41, no. 13, p. 6281-6289. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.06.053> Typ: ADCA

## 5.) Príprava a charakterizácia granúl / mikroguličiek na báze nitridu kremičitého pre bioaplikácie (Preparation and characterization granuls/microspheres based on silicon nitride for bioapplications)

<b>Zodpovedný riešiteľ:</b>	Miroslav Hnatko
<b>Trvanie projektu:</b>	1.1.2018 / 31.12.2021
<b>Evidenčné číslo projektu:</b>	2/0152/18
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	0
<b>Čerpané financie:</b>	SAV: 7351 €

### Dosiahnuté výsledky:

V poslednej etape projektu bola úspešne zvládnuta príprava kompozitných materiálov na báze kalcium-fosfátových cementov s prídavkom pórovitých SN mikroguličiek. Bola zvládnuta charakterizácia pripravených kompozitov z hľadiska stanovenia mechanických vlastností, času tuhnutia, resorbovateľnosti a biologických vlastností pripravených kompozitov. V kompozitných materiáloch bolo zaznamenané zrýchlenie uvoľňovania dexamethasonu, čo je predpokladom úspešného využitia v kontrolovanom rozpúšťaní liečiv.

Publikácie:

MEDVECKÝ, Ľubomír - ŠTULAJTEROVÁ, Radoslava - GIRETOVÁ, Mária - SOPČÁK, Tibor - FÁBEROVÁ, Mária - HNATKO, Miroslav - FENCLOVÁ, Taťána. Calcium phosphate cement modified with silicon nitride/tricalcium phosphate microgranules. In Powder Metallurgy Progress: Journal of Science and Technology of Particle Materials, 2020, vol. 20, no. 1, p. 56-75. Dostupné na: <https://doi.org/10.2478/pmp-2020-0006>

## 6.) Korózia a zvetrávanie úžitkových skiel (Corrosion and weathering of tableware glass)

<b>Zodpovedný riešiteľ:</b>	Mária Chromčíková
<b>Trvanie projektu:</b>	1.1.2018 / 31.12.2021
<b>Evidenčné číslo projektu:</b>	1/0064/18
<b>Organizácia je koordinátorom projektu:</b>	nie
<b>Koordinátor:</b>	Trenčianska univerzita Alexandra Dubčeka v Trenčíne
<b>Počet spoluriešiteľských inštitúcií:</b>	0
<b>Čerpané financie:</b>	VEGA MŠ: 2703 €

### Dosiahnuté výsledky:

Povrchové napätie 14 skiel so zložením odvodeným od bárnateho krištáľového skla (10,49 Na<sub>2</sub>O - 2,36 K<sub>2</sub>O - 9,06 CaO - 0,78 ZnO - 2,44 BaO - 0,85 Al<sub>2</sub>O<sub>3</sub> - 74,02 SiO<sub>2</sub>) bolo opísané ako multilineárna funkcia rovnovážneho moláru množstvo komponentov termodynamického modelu Shakhmatkina a Vedishcheva (SVTDM). Na tomto základe SiO<sub>2</sub> a

$\text{Na}_2\text{O} \cdot 2\text{CaO} \cdot 3\text{SiO}_2$  boli identifikované ako povrchovo najaktívnejšie komponent. V dôsledku silných pozitívnych korelácií medzi rovnovážnymi molárnymi množstvami komponenty SVTDM aj ďalšie komponenty sú identifikované ako pravdepodobne povrchovo aktívne. Získané výsledky sú v zhode s povrchovo aktívnymi oxidmi ( $\text{Na}_2\text{O}$ ,  $\text{K}_2\text{O}$ ,  $\text{ZnO}$ ,  $\text{Al}_2\text{O}_3$  a  $\text{SiO}_2$ ) stanovené na základe závislosti povrchového napätia od oxidovej skloviny zloženie.

The surface tension of 14 glasses with a composition derived from barium crystal glass (10.49  $\text{Na}_2\text{O}$  - 2.36  $\text{K}_2\text{O}$  - 9.06  $\text{CaO}$  - 0.78  $\text{ZnO}$  - 2.44  $\text{BaO}$  - 0.85  $\text{Al}_2\text{O}_3$  - 74.02  $\text{SiO}_2$ ) was described as the multilinear equilibrium molar function of a number of components of the Shakhmatkin and Vedishchev thermodynamic model (SVTDM). On this basis,  $\text{SiO}_2$ , and  $\text{Na}_2\text{O} - 2\text{CaO} - 3\text{SiO}_2$  were identified as the most surface-active components. Due to the strong positive correlations between the equilibrium molar amounts, the SVTDM components and other components are identified as likely to be surfactants. The obtained results are determined in accordance with the surfactant oxides ( $\text{Na}_2\text{O}$ ,  $\text{K}_2\text{O}$ ,  $\text{ZnO}$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{SiO}_2$ ) because of the dependence of the surface tension on the oxide glass composition.

## 7.) Štruktúra a vlastnosti bio aktívnych skiel dopovaných iónmi s potenciálne terapeutickými a antibakteriálnymi účinkami (*Structure and properties of bioactive glasses doped with ions with potential therapeutic and antibacterial effects*)

<b>Zodpovedný riešiteľ:</b>	Mária Chromčíková
<b>Trvanie projektu:</b>	1.1.2020 / 31.12.2023
<b>Evidenčné číslo projektu:</b>	2/0164/
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	1 - Slovensko: 1
<b>Čerpané financie:</b>	SAV: 594 €

### Dosiahnuté výsledky:

Zistilo sa, že zvyšujúci sa obsah  $\text{Li}_2\text{O}$  výrazne znižuje charakteristické teploty spojené s kinetikou skleného prechodu - dilatometrické ako aj kalorimetrické hodnoty teploty skleného prechodu  $T_g$ . Opačný efekt (niekoľkokrát silnejší v pomere k mol. %) bol identifikovaný pre obsah  $\text{P}_2\text{O}_5$ . Na stanovenie parametrov TNM  $\gamma$  a  $x$  bola použitá simulačná porovnávacia metóda; výkonnosť metódy bola analyzovaná s ohľadom na vplyv experimentálne stanovenej aktivačnej energie štruktúrálnej relaxácie  $\gamma^*$ . Vzhľadom na to, že sa zistilo, že hodnoty  $\gamma^*$  sledujú podobný vzor závislosti od oxidov  $\text{P}_2\text{O}_5$  a  $\text{Li}_2\text{O}$ , zdá sa, že vývoj parametrov  $\gamma$  a  $x$  TNM je takmer výlučne riadený obsahom  $\text{P}_2\text{O}_5$ .

It was found that the increasing content of  $\text{Li}_2\text{O}$  significantly reduces the characteristic temperatures with the kinetics of the associated glass transition - dilatometric as well as calorimetric values of the glass transition temperature  $T_g$ . The opposite effect (several times exactly relative to mol%) was identified for the  $\text{P}_2\text{O}_5$  content. A simulation comparison method was used to determine the TNM  $\gamma$  and  $x$  parameters; the performance of the method was analyzed with respect to the influence of experimentally determined activation energy of structural relaxation  $\gamma^*$ . Given that  $\gamma^*$  values have been found to follow a similar pattern of  $\text{P}_2\text{O}_5$  and  $\text{Li}_2\text{O}$  oxides, the development of  $\gamma$  and  $x$  TNM parameters appears to be almost intrinsic to the controlled  $\text{P}_2\text{O}_5$  content.

## 8.) Fotoluminiscenčné transparentné keramické materiály na báze oxinitridov (*Photoluminescent transparent oxynitride-based ceramics*)

<b>Zodpovedný riešiteľ:</b>	Zoltán Lenčes
<b>Trvanie projektu:</b>	1.1.2018 / 31.12.2021
<b>Evidenčné číslo projektu:</b>	2/0164/18
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	0
<b>Čerpané financie:</b>	SAV: 10397 €

### Dosiahnuté výsledky:

Nadalej bol študovaný vplyv množstva lantanoidov (Eu, Ce, Sm, Er) v koncentráciách 0,25 mol%, 0,15 mol% a 0,10 mol% na luminiscenčné vlastnosti oxinitridového spinelu  $\text{MgAlON}$  (tuhý roztok  $\text{MgAl}_2\text{O}_4$  a  $\text{AlN}$ ). V prípade dopantov Eu, Ce a Sm sa intenzita emitovaného žiarenia zvyšovala so zvyšujúcim sa obsahom lantanoidu, kým v prípade luminoforov dopovaných Er bola dosiahnutá maximálna luminiscencia pre vzorku s najnižším obsahom dopantu (0,10



mol% Er). Maximá emisných spektier po excitácii 350 nm žiarením boli v oblasti 570 nm (zeleno-žlté) pre MgAlON:Ce, 670 nm (červené) pre MgAlON:Sm, 470 nm (modré svetlo) pre vzorky MgAlON:Eu a 450 nm (modré) pre MgAlON:Er.

Za účelom fotokatalytických aplikácií boli na transparentnom oxidovom spineli  $\text{MgAl}_2\text{O}_4$  a translucenčnom oxinitridovom spineli MgAlON pripravené  $\text{TiO}_2$  nanorúrky anodickou oxidáciou titánovej vrstvičky nanosené na tieto keramické podložky. Fotokatalytické testy ukázali dobrú účinnosť odstraňovania polutantov (rhodamínu B a bisphenolu A) z vody pomocou  $\text{TiO}_2$  nanorúrok aktivovaných UVA žiarením na transparentných/translucenčných spineloch.

Bola študovaná aj tepelná vodivosť vzoriek MgAlON (so zložením  $\text{Mg}_{0.225}\text{Al}_{1.325}\text{O}_{1.875}\text{N}_{0.225}$ ) a kompozitu 70 hm% MgAlON + 30 hm% AlN. Po spekaní vzoriek pri 1700 °C po dobu 15 min v rapid hot-press bola dosiahnutá tepelná vodivosť 12 W/m·K (doposiaľ najvyššia publikovaná hodnota tepelnej vodivosti MgAlON je 9 W/m·K). Po následnom žiahaní vzoriek pri 1680 °C v pretlaku dusíka (1 MPa) po dobu 12 h za účelom rastu zŕn a odstránenia defektov (vakancií) sa podarilo dosiahnuť tepelnú vodivosť 17 W/m·K.

Publikácie:

1. PETRISKOVÁ, Patrícia - MONFORT, O. - SATRAPINSKY, Leonid - DOBROČKA, Edmund - PLECENIK, T. - PLESCH, Gustáv - PAPŠÍK, Roman - BERMEJO, Raúl - LENČEŠ, Zoltán\*\*. Preparation and photocatalytic activity of  $\text{TiO}_2$  nanotube arrays prepared on transparent spinel substrate. In *Ceramics International*, 2021, vol. 47, no. 9, p. 12970-12980.
2. PETRISKOVÁ, Patrícia – MONFORT, Olivier – LENČEŠ, Zoltán – SATRAPINSKY, Leonid – PLESCH, Gustav. Preparation of  $\text{TiO}_2$  nanotube arrays on transparent spinel for photocatalytic applications. In *Conference Proceedings, Book of extended abstracts from Processing and Properties of Advanced Ceramics and Glasses 2020*, Trenčín, Slovakia. Ed. Vanda Mokránová, reviewers: J. Dusza, D. Galusek, M. Liška, M. Hnatko, P. Hvizdoš, Z. Lenčes, F. Lofaj. Published by FunGlass – Centre for Functional and Surface Functionalized Glass, Trenčín, 2020, pp. 30-31. ISBN 978-80-570-2636-5.

## 9.) Pokrok vo výpočte a interpretácii spektroskopických parametrov zlúčenín ťažkých prvkov (*Advancing in calculation and interpretation of spectroscopic parameters of heavy element compounds*)

**Zodpovedný riešiteľ:**

Oľga Malkin

**Trvanie projektu:**

1.1.2021 / 31.12.2024

**Evidenčné číslo projektu:**

2/0135/21

**Organizácia je koordinátorom projektu:**

áno

**Koordinátor:**

Ústav anorganickej chémie SAV

**Počet spoluriešiteľských inštitúcií:**

0

**Čerpané financie:**

SAV: 15869 €

### Dosiahnuté výsledky:

Boli vyvinuté prístupy na analýzu viacerých spin-spinových väzobných dráh v komplexných systémoch vrátane komplexov prechodných kovov a aplikované na niekoľko systémov. Zodpovedajúci rukopis je v záverečnej fáze prípravy.

## 10.) Vývoj a charakterizácia sférických mikročastíc vhodných na prípravu 3D sklených a sklo-keramických štruktúr (*Development and characterisation of spherical microparticles for preparation of advanced 3D glass and glass-ceramic structures*)

**Zodpovedný riešiteľ:**

Monika Micháľková

**Trvanie projektu:**

1.1.2020 / 31.12.2023

**Evidenčné číslo projektu:**

1/0456/20

**Organizácia je koordinátorom projektu:**

nie

**Koordinátor:**

Ústav anorganickej chémie SAV

**Počet spoluriešiteľských inštitúcií:**

0

**Čerpané financie:**

VEGA MŠ: 2316 €

### Dosiahnuté výsledky:

Nové výrobné techniky, ako je aditívna výroba označovaná aj ako 3D tlač, zohrávajú rozhodujúcu úlohu pri príprave nových bioaktívnych trojrozmerných sklokeramických skeletov. Práca sa zameriava na použitie Ca-Mg silikátových mikrogulôčiek ( $\text{Ca}_2\text{MgSi}_2\text{O}_7$ , t. j. 40 mol % CaO, 20 % MgO a 40 %  $\text{SiO}_2$ ) na výrobu 3D štruktúr aditívnou výrobou. V prvom kroku sa predišlo kryštalizácii kermanitového systému tým, že sa takmer úplne vykryštalizované prekurzorové prášky pripravené konvenčným kalením taveniny vložili do kyslíkovo-metánového ( $\text{O}_2/\text{CH}_4$ ) horáka a pripravili sa plné sklenené mikrogulôčky (SGM) s priemerom pod 63  $\mu\text{m}$ . V druhom kroku sa kryštalizácia využila na kontrolu viskózneho toku SGMs počas vypaľovania sieťovaných skeletov, ktoré sa získali digitálnym svetelným spracovaním (DLP) SGMs

rozdispergovaných vo fotokurabilnom akrylátovom spojive. Sférický tvar umožnil vysoký obsah pevnej látky - až 77 hmotn % SGM v suspenzii. Po vypálení organického spojiva viedlo rýchle spekanie pri teplote 950 °C počas 30 minút k vytvoreniu skeletov, ktoré si zachovali makroporéznosť z modelu 3D tlače (diamantová bunková mriežka), ale s dobre zhutnenými vzperami. Kryštalizácia 3D skeletov počas spekania viedla k vzniku 3D štruktúr s primeraným pomerom pevnosti a hustoty.

**11.) Potenciál vrstevnatých aluminosilikátov ako excelentných nosičov polykatiónov: dizajnovanie nových kompozitných nanomateriálov** (*Potential of layered aluminosilicates as excellent guests to accommodate polymeric cations: design of new composite materials*)

**Zodpovedný riešiteľ:** Helena Pálková  
**Trvanie projektu:** 1.1.2021 / 31.12.2024  
**Evidenčné číslo projektu:** 2/0166/21  
**Organizácia je koordinátorom projektu:** áno  
**Koordinátor:** Ústav anorganickej chémie SAV  
**Počet spoluriešiteľských inštitúcií:** 0  
**Čerpané financie:** SAV: 17853 €

Dosiahnuté výsledky:

V prvom roku riešenia projektu sa pripravili formy ílových minerálov zo skupiny smektitov modifikované polykatiónmami zo skupiny polyoxazolínov a polyetylimínov. Boli pripravené série vzoriek s postupne narastajúcim obsahom organickej fázy. V ďalšej etape sa budú detailnejšie analyzovať vzorky pomocou IČ spektroskopie, termickej analýzy a rtg difrakčnej analýzy.

Publikácie:

1. PÁLKOVÁ, Helena\*\* - BARLOG, Martin - MADEJOVÁ, Jana - HRONSKÝ, V. - PETRA, L. - ŠIMON, Erik - BILLIK, Peter - ZIMOWSKA, M. Structural changes in smectites subjected to mechanochemical activation: The effect of the occupancy of the octahedral sites. In Applied Clay Science, 2021, vol. 213, p. 106214. (2020: 5.467 - IF, Q1 - JCR) 10.1016/j.clay.2021.106214 Typ: ADCA
2. ŠIMONOVÁ, Tímea\*\* - MÉSZÁROS, R. - SEBECHLEBSKÁ, Táňa - BUJDÁK, Juraj\*\*. Non-Arrhenius kinetics and slowed-diffusion mechanism of molecular aggregation of a rhodamine dye on colloidal particles. In Physical Chemistry Chemical Physics, 2021, vol. 23, no. 32, p. 17177-17185. (2020: 3.676 - IF, Q1 - JCR, 1.053 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 1463-9076. Dostupné na: <https://doi.org/10.1039/d1cp02762j> Typ: ADCA
3. ZHOU, Ling - SLANÝ, Michal\* - BAI, Bingbing - DU, Weichao - QU, Chengtun - ZHANG, Jie - TANG, Ying\*\*. Enhanced removal of sulfonated lignite from oil wastewater with multidimensional MgAl-LDH nanoparticles. In Nanomaterials-Basel, 2021, vol. 11, no. 4, p. 861-1-861-18. (2020: 5.076 - IF, Q1 - JCR, 0.919 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents, WOS, SCOPUS). ISSN 2079-4991. Dostupné na: <https://doi.org/10.3390/nano11040861> Typ: ADCA

**12.) Porozumenie mechanizmu interakcií znečisťujúcich látok adsorbovaných na povrchu aluminosilikátových štruktúr** (*Insight into the mechanism of interactions of pollutants adsorbed on the surface of aluminosilicate structures*)

**Zodpovedný riešiteľ:** Eva Scholtzová  
**Trvanie projektu:** 1.1.2019 / 31.12.2022  
**Evidenčné číslo projektu:** 2/0021/19  
**Organizácia je koordinátorom projektu:** áno  
**Koordinátor:** Ústav anorganickej chémie SAV  
**Počet spoluriešiteľských inštitúcií:** 0  
**Čerpané financie:** SAV: 8926 €

Dosiahnuté výsledky:

Štúdium interakcií organických surfaktantov ako aj herbicídov atrazínu a diurónu s povrchom motmorilonitu a beidellitu teoretickým modelovaním ukázalo, že prítomnosť organického surfaktantu výrazne napomáha štruktúrnej stabilite a adsorpcii oboch herbicídov, pri čom hybridné komplexy na báze beidellite sú štruktúrne stabilnejšie ako na báze motmorilonitu. Taktiež bola použitím modelovania a ab initio DFT metódy spresnená kryštálová štruktúra hektoritu

interkalovaného TMA katiónmi, čo nebolo možné dosiahnuť experimentálnym meraním.

Výstupy:

1. MORENO RODRÍGUEZ, Daniel\*\* – JANKOVIČ, Ľuboš – SCHOLTZOVÁ, Eva – TUNEGA, Daniel. Stability of atrazine-smectite intercalates: Density functional theory and experimental study. In MINERALS-BASEL, 2021, vol. 11, no. 6, p. 554-1-554-20. (2020: 2.644 – IF) ADCA
2. JANKOVIČ, Ľuboš\*\* – ŠKORŇA, Peter – MORENO RODRÍGUEZ, Daniel – SCHOLTZOVÁ, Eva – TUNEGA, Daniel. Preparation, characterization and adsorption properties of tetraalkylphosphonium organobidellites. In Applied Clay Science, 2021, vol. 204, p. 105989-1-105989-10. (2020: 5.467 – IF) Typ: ADCA
3. SCHOLTZOVÁ, Eva\*\*. Insight into the structure of TMA-hectorite: A theoretical approach. In MINERALS-BASEL, 2021, vol. 11, no. 5, p. 505-1-505-11. (2020: 2.644 – IF) ADCA
4. MORENO RODRÍGUEZ, Daniel – JANKOVIČ, Ľuboš – SCHOLTZOVÁ, Eva. Taking a look at the interactions between diuron and smectite. In 8th Workshop of Slovak Clay Group. Clay Minerals and Selected Industrial Minerals in Material Science, Applications and Environmental Technology, September 6-8, 2021, Habovka, Slovakia: Book of abstracts. Slovak Clay Group, 2021, p. 21-22. ISBN 978-80-972367-5-5. Typ: AFH

### 13.) Fluoridové taveninové systémy s potenciálom využitia v elektrochemickej výrobe hliníka (*Fluoride melts with potential applications in electrochemical aluminum production*)

<b>Zodpovedný riešiteľ:</b>	František Šimko
<b>Trvanie projektu:</b>	1.1.2018 / 31.12.2021
<b>Evidenčné číslo projektu:</b>	2/0060/18
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	0
<b>Čerpané financie:</b>	SAV: 10414 €

#### Dosiahnuté výsledky:

Uskutočnila sa príprava zlúčenín zaujímavých pre nové, „nízkotaviteľné“ kvapalné elektrolyty v elektrometalurgii, ako aj pre rôzne elektronické a fotonické aplikácie (tuhé elektrolyty, scintilátory). Dané využitie súvisí so štruktúrou hexafluórohlinitanu rubídneho,  $\text{Rb}_3\text{AlF}_6$ . Tá patrí do veľmi úzkej skupiny štruktúry zdvojeného perovskytu, ktorá vykazuje ne-kooperatívne nakláňanie oktaédrických štruktúrnych jednotiek (non-cooperative octahedral tilting - NCOT). Preto sa uskutočnila štruktúrna charakterizácia danej komplexnej zlúčeniny. Pomocou synchrotronovej práškovej štruktúrnej analýzy spojenej s viacjadrovou solid state NMR spektroskopiou v tuhom stave, doplnených o TEM analýzy a DFT výpočty sa dokázala prítomnosť dvoch rozdielnych polymorfných foriem  $\text{Rb}_3\text{AlF}_6$ . Prvá je  $\alpha$ -fáza, existujúca pri izbovej teplote, ktorá kryštalizuje v priestorovej grupe  $Fddd$  s parametrami základnej bunky  $a = 37.26491(1) \text{ \AA}$ ,  $b = 12.45405(4) \text{ \AA}$ ,  $c = 17.68341(6) \text{ \AA}$ . Tá je práve súčasťou malej skupiny zlúčenín s ne-kooperatívnym nakláňaním oktaédrických jednotiek v ich štruktúre. Použitie in-situ vysokoteplotnej MAS NMR analýzy bolo výhodné pre sledovanie chemických zmien v štruktúre  $\text{Rb}_3\text{AlF}_6$  so zvyšujúcou sa teplotou. Pri vyššej teplote (nad  $600^\circ\text{C}$ ) sa určila prítomnosť vysokoteplotnej, polymorfnéj  $\beta$ -fázy, ktorá existuje ako kubická, dvojité-perovskitická štruktúra s priestorovou grupou  $Fm\bar{3}m$ , s parametrami základnej bunky  $a = 8.9930(2) \text{ \AA}$ .

Spojenie 1D a 2D NMR techník v tuhom stave vrátane in-situ vysokoteplotnej MAS NMR analýzy spolu s elektrónovou a synchrotronovou práškovou difrakciou bolo prvýkrát použité pre určenie tak zložitej štruktúry.

## Programy: APVV

### 14.) Interakcia fluoridových taveninových systémov prvkov vzácnych zemín s oxidmi kritických prvkov v kontexte špeciálnych aplikácií (*Interaction of fluoride melts of rare earth elements with oxides of critical elements in the context of special applications*)

<b>Zodpovedný riešiteľ:</b>	Miroslav Boča
<b>Trvanie projektu:</b>	1.7.2020 / 30.6.2024
<b>Evidenčné číslo projektu:</b>	APVV-19-0270
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	0

**Čerpané financie:**

APVV: 70000 €

Dosiahnuté výsledky:

Difrakčná a luminiscenčná analýza vzoriek  $(\text{LiF}-\text{CaF}_2)_{\text{eut}}-\text{xSmF}_3(-\text{xGdF}_3)$  ukázala, že LiF stabilizuje kubickú bunku a obsah  $\text{LnF}_3$  vplyva na prítomné fázy, kryštalinitu sústavy i . fotoluminiscenčné vlastnosti. Mechanické roztretie zvyšuje luminiscenčné vlastnosti a vedie k vyššej intenzite emisie. Experimenty ukázali, že fotoluminiscenčná spektroskopia je vhodná na detekciu/potvrdenie zníženia lokálnej symetrie na základerozdelenia spektrálnych pásov.

## Výstupy:

BOČA, Miroslav\*\* - MLYNÁRIKOVÁ, Jarmila - MACKOVÁ, Iveta - JANIČKOVIČ, Dušan - CZÍMEROVÁ, Adriana - SHI, Zhongning. Diffraction and luminescence analysis of extremely rapidly cooled molten system  $(\text{LiF}-\text{CaF}_2)_{\text{eut}}-\text{xLnF}_3$  ( $\text{Ln}=\text{Sm}$  and  $\text{Gd}$ ). In Transactions of Nonferrous Metals Society of China, 2021, vol. 31, no. 4, p. 1151-1164. (2020: 2.917 - IF, Q1 - JCR, 0.744 - SJR, Q1 - SJR). ISSN 1003-6326.

**15.) Nové sklenené a sklokeramické fosfory na báze hlinitanov vzácnych zemín pre aplikácie v pevnolátkových energií šetriacich svetelných zdrojoch vyžarujúcich biele svetlo (pc-ELED diódy)**  
*(Novel glass and glass-ceramic rare-earth aluminates-based phosphors for energy-savin solid state lighting sources emitting while light (pc-WLEDs))*

**Zodpovedný riešiteľ:**

Dušan Galusek

**Trvanie projektu:**

1.8.2018 / 31.7.2022

**Evidenčné číslo projektu:**

APVV-17-0049

**Organizácia je koordinátorom projektu:**

nie

**Koordinátor:**

Trenčianska univerzita Alexandra Dubčeka v Trenčíne

**Počet spoluriešiteľských inštitúcií:**

0

**Čerpané financie:**

APVV: 12060 €

Dosiahnuté výsledky:

Optimalizovala sa príprava mikrogulôčok v systéme  $\text{Y}_2\text{O}_3-\text{Al}_2\text{O}_3$  dopovanom luminiscenčne aktívnymi iónmi  $\text{Ce}^{3+}$ ,  $\text{Eu}^{3+}/^{2+}$ ,  $\text{Mn}^{2+}/^{4+}$ . Detailne sa preštudovali luminiscenčné vlastnosti v závislosti od koncentrácie aktivátora, podmienok prípravy skryštalizovaných mikrogulôčok (optimalizovaný časovo-teplotný režim v redukčnej atmosfére).  $\text{Eu}^{2+}$  - dopované systémy vykazujú pri excitácii NUV emisiu bieleho svetla, ktorú je možno ladiť vlnovou dĺžkou excitačného žiarenia s posunom do červenej spektrálnej oblasti. Z  $\text{Ce}^{3+}$  dopovaných sklenených mikrogulôčok boli žiarovým lisovaním pripravené sklo-kryštalické dvojfázové ( $\text{YAG}/\text{Al}_2\text{O}_3$ ) translucenčné kompakty s luminiscenčnými vlastnosťami, ktoré emitujú žlté svetlo pri excitácii NUV a modrým svetelným žiarením. Žiarovým lisovaním boli pripravené aj kompozity dopované  $\text{Eu}^{2+}/\text{Eu}^{3+}$  emitujúce biele svetlo pri excitácii NUV iba s jedným typom aktivátora v matici.

## Výstupy:

1. KLEMENT, Róbert\*\* - DRDLÍKOVÁ, K. - KACHLÍK, M. - DRDLÍK, Daniel - GALUSEK, Dušan - MACA, Karel. Photoluminescence and optical properties of  $\text{Eu}^{3+}/\text{Eu}^{2+}$ -doped transparent  $\text{Al}_2\text{O}_3$  ceramics. In Journal of the European Ceramic Society, 2021, vol. 41, no. 9, p. 4896-4906.
2. AKUSEVICH, A. – PARCHOVIANSKA, R – PARCHOVIANSKÝ M. – PRNOVÁ A. – LOFAJ F. – VOJTKO M. – KLEMENT R. Glass-ceramic  $\text{Ce}^{3+}$ -doped  $\text{YAG}-\text{Al}_2\text{O}_3$  composites prepared by sintering of glass microspheres, International Journal of Applied Glass Science, 12 (2021) 497-508.

**16.) Nanoštrukturované, funkčne navrstvené a bio-inšpirované 3D iplantáty na báze titánu**  
*(Nanostructured, functionally graded, and bioinspired 3D Ti-based implants)*

**Zodpovedný riešiteľ:**

Miroslav Hnatko

**Trvanie projektu:**

1.8.2021 / 30.6.2025

**Evidenčné číslo projektu:**

APVV-20-0322

**Organizácia je koordinátorom projektu:**

áno

**Koordinátor:**

Ústav anorganickej chémie SAV

**Počet spoluriešiteľských inštitúcií:** 1 - Slovensko: 1  
**Čerpané financie:** APVV: 14750 €

Dosiahnuté výsledky:

V súlade s harmonogramom bola v spolupráci s firmou Biomedical Engineering s.r.o. navrhnutá a začatá výroba (3D tlač) prvých substrátov na báze titánu. Následne bol posúdený vplyv povrchovej úpravy 3D výrobkov pieskovaním (rôznymi médiami), na konečnú morfológiu povrchu a na mieru chemickej kontaminácie. Boli vykonané prvé experimenty s cieľom: i.) zistiť vplyv elektrochemickej úpravy povrchu substrátov, ii.) optimalizovať process anodickej oxidácie povrchu s cieľom vytvoriť trojrozmernú nanotubulárnu vrstvu TiO<sub>2</sub>, iii.) optimalizovať prípravu bioaktívnych skiel na báze bioaktívneho skla 45S5.

**17.) Nové vysoko-entropické keramické materiály pre pokročilé aplikácie** (*New High - Entropy Ceramics for Advanced Applications*)

**Zodpovedný riešiteľ:** Pavol Hvizdoš  
**Zodpovedný riešiteľ v organizácii SAV:** Pavol Šajgalík  
**Trvanie projektu:** 1.7.2020 / 30.6.2024  
**Evidenčné číslo projektu:** APPV-19-0497  
**Organizácia je koordinátorom projektu:** nie  
**Koordinátor:** Ústav materiálového výskumu SAV  
**Počet spoluriešiteľských inštitúcií:** 0  
**Čerpané financie:** APVV: 18500 €

Dosiahnuté výsledky:

Riešenie projektu bolo zamerané na prípravu a charakterizáciu päťzložkových vysoko-entropických karbidov, na báze (Hf-Ta-Zr-Nb-Ti)C a (Mo-Ta-Nb-W-V)C. Oba materiálové systémy boli pripravené homogenizáciou piatich monokarbidických práškov v ekvimolárnom pomere, ktoré boli následne zhutnené pomocou metódy spekania za asistencie elektrického prúdu. V prípade (Hf-Ta-Zr-Nb-Ti)C boli plne hutné materiály pripravené spekaním pri teplote 2050°C a tlaku 70 MPa, zatiaľ čo teplota 1600°C a tlak 70 MPa boli postačujúce na získanie plne hutných (Mo-Ta-Nb-W-V)C materiálov. V oboch prípadoch sa podarilo pripraviť homogénny materiál s prítomnosťou jednofázového tuhého roztoku. Pomocou RTG analýzy sa určili mriežkové parametre kryštálovej mriežky u všetkých vzoriek. Stanovili sa mechanické vlastnosti pri izbovej teplote, t.j. tvrdosť, elastický modul, lomová húževnatosť, ako aj odolnosť proti opotrebeniu. Bolo preukázané, že tvrdosť a elastický modul hraníc zŕn je približne o 8% nižšia ako tvrdosť a elastický modul samotných zŕn HEC materiálov.

Výstupy:

DUSZA, Ján - CSANÁDI, Tamás\*\* - MEDVEĎ, Dávid - SEDLÁK, Richard - VOJTKO, Marek - IVOR, Michal - ŮNSAL, Hakan - TATARKO, Peter - TATARKOVÁ, Monika - ŠAJGALÍK, Pavol. Nanoindentation and tribology of a (Hf-Ta-Zr-Nb-Ti)C high-entropy carbide. In Journal of the European Ceramic Society, 2021, vol. 41, no. 11, p. 5417-5426. (2020: 5.302 - IF, Q1 - JCR). Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.05.002>

**18.) Bentonit: strategická surovina Slovenska - inovatívne hodnotenie zdrojov a ich kvality pre jej efektívne využívanie** (*Bentonite: Slovak strategic raw material - Innovative assessment of bentonite quality and origin for its efficient use*)

**Zodpovedný riešiteľ:** Jana Madejová  
**Trvanie projektu:** 1.1.2021 / 30.6.2025  
**Evidenčné číslo projektu:** APVV-20-0175  
**Organizácia je koordinátorom projektu:** nie  
**Koordinátor:** Univerzita Komenského v Bratislave  
**Počet spoluriešiteľských inštitúcií:** 0  
**Čerpané financie:** APVV: 3550 €

Dosiahnuté výsledky:

V prvom polroku riešenia projektu bol realizovaný odber vzoriek bentonitov z vybraných ložísk. Separáciou sa získali hrobozrné frakcie <0.25 mm a jemnozrné frakcie <0.25 μm. Na získanie informácií o minerálnom a chemickom zložení bentonitov sa využila aj IČ spektroskopia. Kvalitný bentonit s hlavným minerálom montmorillonitom a minimálnym množstvom prímies bol potvrdený pre lokalitu Lutila, v prípade bentonitu z lokality Stará Kremnička bol vo vzorke okrem

montmorillonitu identifikovaný aj cristobalit a kaolinit.

**19.) Bionanokompozitné materiály na báze vrstevnatých silikátov** (*Bionanocomposites based on organic polycations and layered silicates*)

**Zodpovedný riešiteľ:** Jana Madejová  
**Trvanie projektu:** 1.7.2020 / 30.6.2024  
**Evidenčné číslo projektu:** APVV-19-0487  
**Organizácia je koordinátorom projektu:** áno  
**Koordinátor:** Ústav anorganickej chémie SAV  
**Počet spoluriešiteľských inštitúcií:** 0  
**Čerpané financie:** APVV: 32100 €

Dosiahnuté výsledky:

V druhom roku riešenia projektu bol výskum zameraný na prípravu a charakterizáciu vzoriek montmorillonitu (Mt) modifikovaného rôznymi typmi polymérov. Pripravili sa série organoílov z Na-Mt Kunipia a neiónového polyméru poly(2-metyl-2-oxazolín) (PMeOx-Mt) a kationového polyméru polyetylénimín (PEI-Mt). Začala sa ich komplexná charakterizácia pomocou RTG, TG a IČ spektroskopie v strednej aj blízkej oblasti. Ukázal sa rôzny rozsah interkalácie organickej fázy do medzivrstvových priestorov montmorillonitu v závislosti od množstva polyméru použitého pri príprave vzorky (loading). Kým v prípade PMeOx-Mt ukázala RTG analýza postupný nárast medziurovňovej vzdialenosti (d001) Mt v závislosti od loading, v prípade PEI-Mt bolo množstvo PEI schopné interkalovať sa do medzivrstvových priestorov Mt je obmedzené a pri vyšších loadingoch sa polycation adsorboval na vonkajšie porchy Mt. V prípade PMeOx-Mt sa pomocou ab initio DFT metódy v tuhej fáze uskutočnili výpočty interkalačnej energie zamerané na určenie stability PMeOx-Mt. Paralelne pokračoval aj výskum zameraný na kompozitné materiály pripravené zo smektitov modifikovaných alkylamóniovými, alkyfosfóniovými a PDDA kationmi a fluorescečnými farbivami.

**20.) Vývoj nástrojov pre pokročilú analýzu a predikciu parametrov spektier EPR, NMR a pNMR komplexných systémov obsahujúcich ťažké prvky** (*Development of tools for advanced analysis and prediction of parameters of EPR, NMR and pNMR spectra of complex systems containing heavy elements*)

**Zodpovedný riešiteľ:** Oľga Malkin  
**Trvanie projektu:** 1.7.2020 / 30.6.2024  
**Evidenčné číslo projektu:** APVV-19-0516  
**Organizácia je koordinátorom projektu:** áno  
**Koordinátor:** Ústav anorganickej chémie SAV  
**Počet spoluriešiteľských inštitúcií:** 0  
**Čerpané financie:** APVV: 35763 €

Dosiahnuté výsledky:

1. NOVOTNÝ, Jan\* - JEREMIAS, Lukáš\* - NIMAX, Patrick - KOMOROVSKÝ, Stanislav - HEINMAA, Ivo - MAREK, Radek\*\*. Crystal and substituent effects on paramagnetic NMR shifts in transition-metal complexes. In *Inorganic Chemistry*, 2021, vol. 60, no. 13, p. 9368-9377. (2020: 5.165 - IF) doi.org/10.1021/acs.inorgchem.1c00204
2. DESMARAIS, Jacques K.\*\* - KOMOROVSKÝ, Stanislav - FLAMENT, Jean-Pierre - ERBA, Alessandro. Spin-orbit coupling from a two-component self-consistent approach. II. Non-collinear density functional theories. In *Journal of Chemical Physics*, 2021, vol. 154, no. 20, p. 204110-1-204110-15. (2020: 3.488 - IF) doi.org/10.1063/5.0051447

**21.) Povrchy polymérov modifikované vrstevnatými nanočasticami a fotoaktívnymi farbivami** (*Polymer surfaces modified with layered nanoparticles and photoactive dyes*)

**Zodpovedný riešiteľ:** Helena Pálková  
**Trvanie projektu:** 1.7.2019 / 30.6.2023  
**Evidenčné číslo projektu:** APVV-18-0075  
**Organizácia je koordinátorom projektu:** nie  
**Koordinátor:** Ústav anorganickej chémie SAV  
**Počet spoluriešiteľských inštitúcií:** 0  
**Čerpané financie:** APVV: 25000 €

Dosiahnuté výsledky:

1. BARLOG, Martin\*\* - PÁLKOVÁ, Helena - BUJDÁK, Juraj. Luminescence of a laser dye in organically-modified layered silicate pigments. In Dyes and Pigments, 2021, vol. 191, p. 109380-1-109380-11. (2020: 4.889 - IF, Q1) DADI, Nitin Chandra teja - BUJDÁK, Juraj\*\* - MEDVECKÁ, Veronika - PÁLKOVÁ, Helena - BARLOG, Martin - BUJDÁKOVÁ, Helena\*\*. Surface characterization and anti-biofilm effectiveness of hybrid films of polyurethane functionalized with saponite and phloxine B. In Materials, 2021, vol. 14, no. 14, p. 7583-1-7583-21. (2020: 3.623 - IF, Q1) Typ: ADCA
2. MADEJOVÁ, Jana\*\* - BARLOG, Martin - JANKOVIČ, Ľuboš - SLANÝ, Michal - PÁLKOVÁ, Helena. Comparative study of alkylammonium- and alkylphosphonium-based analogues of organo-montmorillonites. In Applied Clay Science, 2021, vol. 200, p. 105894-1-105894-10. (2020: 5.467 - IF, Q1) Typ: ADCA
3. PÁLKOVÁ, Helena\*\* - BARLOG, Martin - MADEJOVÁ, Jana - HRONSKÝ, V. - PETRA, L. - ŠIMON, Erik - BILLIK, Peter - ZIMOWSKA, M. Structural changes in smectites subjected to mechanochemical activation: The effect of the occupancy of the octahedral sites. In Applied Clay Science, 2021, vol. 213, p. 106214. (2020: 5.467 - IF, Q1) Typ: ADCA
4. BOHÁČ, Peter\*\* - SASAI, Ryo - SOONTORNCHAIYAKUL, W. - CZÍMEROVÁ, Adriana - BUJDÁK, Juraj. Resonance energy transfer between cyanine dyes in hybrid films of layered silicate prepared by layer-by-layer method. In Applied Clay Science, 2021, vol. 202, p. 105985-1-105985-9. (2020: 5.467 - IF, Q1)
5. ŠIMONOVÁ, Tímea\*\* - MÉSZÁROS, R. - SEBECHLEBSKÁ, Táňa - BUJDÁK, Juraj\*\*. Non-Arrhenius kinetics and slowed-diffusion mechanism of molecular aggregation of a rhodamine dye on colloidal particles. In Physical Chemistry Chemical Physics, 2021, vol. 23, no. 32, p. 17177-17185. (2020: 3.676 - IF, Q1) Typ: ADCA

## 22.) Pokročilé materiály s eutektickou mikroštruktúrou pre vysokoteplotné funkčné aplikácie (*Advanced materials with eutectic microstructure for high temperature and functional applications*)

<b>Zodpovedný riešiteľ:</b>	Anna Prnová
<b>Trvanie projektu:</b>	1.7.2020 / 30.6.2024
<b>Evidenčné číslo projektu:</b>	APVV-19-0010
<b>Organizácia je koordinátorom projektu:</b>	nie
<b>Koordinátor:</b>	Trenčianska univerzita Alexandra Dubčeka v Trenčíne
<b>Počet spoluriešiteľských inštitúcií:</b>	1 - Slovensko: 1
<b>Čerpané financie:</b>	APVV: 18115 €

Dosiahnuté výsledky:

V rámci projektu bolo pripravené: 1 sklo v systéme  $\text{Al}_2\text{O}_3\text{-Y}_2\text{O}_3$ , z ktorého boli žiarovým lisovaním a SPS metódou pripravené kusové vzorky s dobrými mechanickými vlastnosťami (výsledky publikované v Pure and Applied chemistry, 2021) ďalej bolo pripravených 5 skiel s odlišným obsahom  $\text{ZrO}_2$  v systéme  $\text{Al}_2\text{O}_3\text{-Y}_2\text{O}_3\text{-ZrO}_2$ , žiarovým lisovaním a SPS syntézou boli pripravené prvé kusové vzorky, pričom jedna vzorka bola translucetná. Termickými analýzami sa skúmalo teplotné správanie sa pripravených systémov a výsledky boli prezentované na SSC konferencii v Trenčíne a na konferencii v Pardubiciach ČR: 23. ročník Konference o speciálních anorganických pigmentech a práškových materiáloch.

## 23.) Anódy pre Li-iónové batérie na báze uhlík-kremíkových kompozitov (*Carbon-silicon based composite anodes for Li-ion batteries*)

<b>Zodpovedný riešiteľ:</b>	Jaroslav Sedláček
<b>Zodpovedný riešiteľ v organizácii SAV:</b>	Zoltán Lenčes
<b>Trvanie projektu:</b>	1.7.2020 / 30.6.2024
<b>Evidenčné číslo projektu:</b>	APPV-19-0461
<b>Organizácia je koordinátorom projektu:</b>	nie
<b>Koordinátor:</b>	Centrum pre využitie pokročilých materiálov SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	3 - Slovensko: 3
<b>Čerpané financie:</b>	APVV: 6392 €

Dosiahnuté výsledky:

Na prípravu anód Li-batérií boli použité zmesi práškov kremíka a uhlíka. Nakoľko má veľkosť častíc prášku vplyv na vlastnosti batérií, bolo nutné optimalizovať podmienky mletia práškov. Za týmto účelom bol zhotovený model (Design of experiment) ktorý umožní odhadnúť vplyv podmienok mletia (rýchlosť otáčania planetového mlynu, čas mletia, pomer prášok/etanol, pomer prášok/mlecie guľičky) na vlastnosti mletého prášku: úroveň kontaminácie prášku mleciami

telieskami, veľkosť kryštálov a veľkosť častíc (rozpätie D10 – D90). Na zhotovenie modelu boli použité výsledky z 19 mletí zmesí práškov Si a C za rôznych podmienok mletia. Na overenie spoľahlivosti modelu sme stanovili požadované vlastnosti mletého prášku nasledovne: úroveň kontaminácie < 1%, veľkosť kryštálov < 40 nm, D10 < 1,5 μm, D90 < 8,1 μm. Pomocou modelových výpočtov boli stanovené podmienky mletia: rýchlosť mletia 320 rpm, čas 12 hod, pomer etanol/prášok = 5, pomer guľičky/prášok = 9,5. Analýza mletých práškov ukázala, že model je spoľahlivý, nakoľko všetky parametre mletých práškov spadali do úzkeho rozpätia plánovaných vlastností.

Boli optimalizované reologické vlastnosti suspenzií Si-C práškov a odliate tenké vrstvy Si-C anód na medenú fóliu. V ochrannnej atmosfére argónu (v glove-boxe) boli zhotovené batérie, pričom elektróda bola lítium a elektrolyt komerčný LiPF<sub>6</sub>. Galvanostatické nabíjacie-vybíjacie testy boli uskutočnené pri rôznych prúdových hustotách (0,2 – 4,0 A/g-1). Výsledky meraní ukázali, že po prvých 3-5 cykloch nabíjania – vybíjania dochádza k prudkému poklesu špecifickej kapacity z 1000 mAh/g na 400 mAh/g. V ostatných cykloch (max. 100 cyklov) dochádzalo k miernemu poklesu kapacity zo 400 mAh/g na cca 200 mAh/g. V ďalších experimentoch bude potrebné optimalizovať hrúbku vrstvy anódy a jej pórovitosť.

## 24.) Vývoj žiaruvzdorných pyrochlórnych fáz pre vysokoteplotné aplikácie neoxidovej keramiky (*Development of refractory pyrochlore phases for high temperature applications of non-oxide ceramics*)

<b>Zodpovedný riešiteľ:</b>	Peter Tatarko
<b>Trvanie projektu:</b>	1.8.2018 / 30.6.2022
<b>Evidenčné číslo projektu:</b>	APVV-17-0328
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	0
<b>Čerpané financie:</b>	APVV: 40441 €

### Dosiahnuté výsledky:

Riešenie projektu bolo zamerané na detailnú charakterizáciu vzoriek ZrB<sub>2</sub>-SiC s rôznym prídavkom pyrochlórnej fázy na báze Yb<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> (2, 5 a 10 hmot.%). Bol pozorovaný minimálny vplyv rôzneho obsahu pyrochlórnej fázy na mechanické vlastnosti materiálov ZrB<sub>2</sub>-SiC, t.j. na tvrdosť, lomovú húževnatosť, Youngov modul pružnosti a pevnosť v ohybe. Získané výsledky boli porovnateľné s mechanickými vlastnosťami materiálu ZrB<sub>2</sub>-SiC s prísadou Yb<sub>2</sub>O<sub>3</sub>, ktoré boli študované v predchádzajúcich etapách projektu. Na rozdiel od mechanických vlastností pri izbovej teplote, odolnosť materiálov proti ablácii pri teplote 2700°C sa výrazne zvyšovala s rastúcim obsahom Yb<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>. Linérna ablačná rýchlosť materiálu obsahujúceho 10 hmot.% Yb<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> bola 3x nižšia ako ablačná rýchlosť referenčného ZrB<sub>2</sub>-SiC materiálu bez prídavku pyrochlórnej fázy. Za najdôležitejší výsledok možno považovať skutočnosť, že prídavkom 10 hmot.% pyrochlórnej fázy došlo k výraznému zlepšeniu odolnosti ZrB<sub>2</sub>-SiC materiálu proti ablácii pri extrémnych teplotách, pričom tento prídavok nespôsobil žiadnu stratu mechanických vlastností pri izbovej teplote.

Časť výskumných aktivít bola tiež venovaná štúdiu spájania keramických kompozitov na báze SiC pre vysokoteplotné aplikácie.

### Výstupy:

1. TATARKO, Peter\*\* - VALENZA, Fabrizio - ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Design of Lu<sub>2</sub>O<sub>3</sub>-reinforced Cf/SiC-ZrB<sub>2</sub>-ZrC ultra-high temperature ceramic matrix composites: Wetting and interfacial reactivity by ZrSi<sub>2</sub> based alloys. In Journal of the European Ceramic Society, 2021, vol. 41, p. 3051-3060. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2020.05.055>
2. ÜNSAL, Hakan - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - TATARKOVÁ, Monika - DLOUHÝ, Ivo - TATARKO, Peter\*\*. In-situ graphene platelets formation and its suppression during reactive spark plasma sintering of boron carbide/titanium diboride composites. In Journal of the European Ceramic Society, 2021, vol. 41, no. 13, p. 6281-6289. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.06.053>
3. SMEACETTO, Federico\*\* - D'ISANTO, Fabiana - CASALEGNO, Valentina - TATARKO, Peter - SALVO, Milena. Ytterbium disilicate-based glass-ceramic as joining material for ceramic matrix composites. In Journal of the European Ceramic Society, 2021, vol. 41, no. 2, p. 1099-1106. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2020.10.022>
4. ZHOU, Xiaobing\*\* - SHI, Linkun - ZOU, Shunrui - XU, Jie - LIU, Yihe - TATARKO, Peter. Fast seamless joining of SiCw/Ti<sub>3</sub>SiC<sub>2</sub> composite using electric field-assisted sintering technique. In International Journal of Applied Ceramic Technology, 2021, vol. 18, no. 5, p. 1670-1676. (2020: 1.968 - IF, Q2 - JCR, 0.400 - SJR, Q2 - SJR). ISSN 1546-542X. Dostupné na: <https://doi.org/10.1111/ijac.13799>
5. ŠKUNDRIĆ, Tamara - MATOVIĆ, Branko - ZARUBICA, Aleksandra - ZAGORAC, Jelena - TATARKO, Peter - ZAGORAC, Dejan\*\*. Structure prediction and mechanical properties of silicon hexaboride on ab initio level. In



Materials, 2021, vol. 14, p. 7887-1-7887-17. (2020: 3.623 - IF, Q1 - JCR, 0.682 - SJR, Q2 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 1996-1944. Dostupné na: <https://doi.org/10.3390/ma14247887>

## 25.) Vývoj bioaktívneho nitridu kremičitého modifikáciou povrchovej vrstvy (*Development of the bioactive silicon nitride by surface modification*)

**Zodpovedný riešiteľ:** Monika Tatarková  
**Trvanie projektu:** 1.7.2019 / 31.12.2022  
**Evidenčné číslo projektu:** APPV-18-0542  
**Organizácia je koordinátorom projektu:** áno  
**Koordinátor:** Ústav anorganickej chémie SAV  
**Počet spoluriešiteľských inštitúcií:** 0  
**Čerpané financie:** APVV: 53825 €

### Dosiahnuté výsledky:

Hutné materiály na báze nitridu kremičitého s rôznym hmotnostným prídavkom  $\text{CaSiO}_3$  a  $\text{Y}_2\text{O}_3$  boli tepelne ovplyvnené kyslíkovo acetylénovým plameňom s cieľom zistiť závislosť teploty plameňa a doby pôsobenia plameňa na tvorbu pórovitej povrchovej vrstvy. Analýzou vytvorenej povrchovej vrstvy, jej hrúbky, chemického zloženia a veľkosti pórov boli zistené najvhodnejšie parametre tepelného ovplyvnenia povrchu experimentálnych vzoriek. Bolo zistené, že pri použitých množstvách spekacích prísad vyššie teploty plameňa pôsobiace kratšiu dobu sú vhodnejšie na tvorbu pórovitej oblasti imitujúcu štruktúru trabekulárnej kosti. Bol zistený výrazný vplyv počiatkovej drsnosti povrchu na tvorbu oxidačnej vrstvy.

### Výstupy:

1. TATARKOVÁ, Monika\*\* - TATARKO, Peter - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - DUSZA, Ján - ŠAJGALÍK, Pavol. Influence of hexagonal boron nitride nanosheets on phase transformation, microstructure evolution and mechanical properties of  $\text{Si}_3\text{N}_4$  ceramics. In Journal of the European Ceramic Society, 2021, vol. 41, no. 10, p. 5115-5126. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR). ISSN 0955-2219. Typ: ADCA. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.01.057>
2. KITYK, A.\*\* - PROTSENKO, V. - DANILOV, F.I. - PAVLÍK, Viliam - HNATKO, Miroslav - ŠOLTÝS, Ján. Enhancement of the surface characteristics of Ti-based biomedical alloy by electropolishing in environmentally friendly deep eutectic solvent (Ethaline). In Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, vol. 613, p. 126125-1-126125-14. (2020: 4.539 - IF, Q2 - JCR, 0.762 - SJR, Q2 - SJR). ISSN 0927-7757. Typ: ADCA. Dostupné na: <https://doi.org/10.1016/j.colsurfa.2020.126125>

## Programy: Štrukturálne fondy EÚ Výskum a inovácie

### 26.) Vybudovanie centra pre využitie pokročilých materiálov SAV (*Building a centre for advanced material application SAS*)

**Zodpovedný riešiteľ:** Eva Majková  
**Zodpovedný riešiteľ v organizácii SAV:** Miroslav Hnatko  
**Trvanie projektu:** 1.7.2019 / 30.6.2023  
**Evidenčné číslo projektu:** NFP313020T081  
**Organizácia je koordinátorom projektu:** nie  
**Koordinátor:** Fyzikálny ústav SAV  
**Počet spoluriešiteľských inštitúcií:** 6 - Slovensko: 6  
**Čerpané financie:** MŠ: 46249 €

### Dosiahnuté výsledky:

V rámci podaktivity 1.4. Pokročilé keramické materiály (milník - príprava anorganicko-organického bioaktívneho kompozitu) sme sa venovali možnosti využitia elektrochemického leštenia zliatiny na báze Ti pomocou ekologicky šetrného rozpúšťadla - etalínu. Ukázalo sa, že elektrolytické leštenie v etaline zaistilo odstránenie povrchových defektov, čím sa zabezpečilo vyhladenie povrchu a zníženie jeho drsnosti. Analýza odhalila, že elektrochemické leštenie titánovej zliatiny v etaline poskytlo tvorbu špecifických vzorov na nanometrovej úrovni s tvarom predĺžených hemisfér. Boli stanovené a diskutované korelácie medzi koeficientmi drsnosti povrchu a parametrami zmáčanlivosti. Boli skúmané

elektrochemické procesy vyskytujúce sa počas elektrochemického leštenia zliatiny na báze Ti v etalíne. Úprava doby spracovania a elektródového potenciálu elektrolytického leštenia umožňuje kontrolovateľne a flexibilne ladiť drsnosť povrchu a zmäčavosť zliatiny obsahujúcej titán.

V rámci tej istej podaktivity bol pri izbovej teplote úspešne zvládnutý aj proces zhutnenia bioaktívneho materiálu (Bioglass®45S5) vo forme prášku (~98 %). Testovala sa zmes Bioglass®45S5 s vodou, alebo s roztokom hydroxidu sodného (1M). Na takúto zmes bol aplikovaný izostatický tlak (400MPa) po dobu 10 minút. Vplyvom hydrostatických podmienok dochádzalo k tvorbe a sekundárnej fázy okolo nerozpustených častíc bioskla. Chemická a fázová analýza preukázala tvorbu C-S-H fázy, pričom Ramanova a <sup>29</sup>Si NMR spektroskopia preukázali, že vzorka spracovaná vo vode má vyššiu konektivitu oxidu kremičitého v porovnaní so vzorkou, kde bol použitý roztok NaOH. Výber rozpúšťadla je rozhodujúci pre rozpúšťanie kationov a aniónov bioskla.

#### Publikácie:

1. KITYK, A.\*\* - HNATKO, Miroslav - PAVLÍK, Viliam - BOČA, Miroslav. Electropolishing of WCu composite in a deep eutectic solvent. In Chemical Papers, 2021, vol. 75, no. 4, p. 1767-1771. (2020: 2.097 - IF, Q3 - JCR, 0.344 - SJR, Q2 - SJR). ISSN 0366-6352. Dostupné na: <https://doi.org/10.1007/s11696-020-01426-5>
2. KITYK, A.\*\* - HNATKO, Miroslav - PAVLÍK, Viliam - BOČA, Miroslav. Electropolishing of WCu composite in a deep eutectic solvent. In Chemical Papers, 2021, vol. 75, no. 4, p. 1767-1771. (2020: 2.097 - IF, Q3 - JCR, 0.344 - SJR, Q2 - SJR). ISSN 0366-6352. Dostupné na: <https://doi.org/10.1007/s11696-020-01426-5>
3. KITYK, A.\*\* - HNATKO, Miroslav - PAVLÍK, Viliam - BOČA, Miroslav. Electrochemical surface treatment of manganese stainless steel using several types of deep eutectic solvents. In Materials Research Bulletin, 2021, vol. 141, p. 111348-1-111348-11. (2020: 4.641 - IF, Q2 - JCR, 0JR). //doi.org/10.1016/j.materresbull.2021.111348
4. TAVERI, Gianmarco\*\* - HANZEL, Ondrej - SEDLÁČEK, Jaroslav - TOUŠEK, Jaromír - NEŠČÁKOVÁ, Z. - MICHÁLEK, Martin - DLOUHÝ, Ivo - HNATKO, Miroslav. Consolidation of Bioglass (R) 45S5 suspension through cold isostatic pressing. In Ceramics International, 2021, vol. 47, no. 3, p. 4090-4096. (2020: 4.527 - IF, Q1 - JCR, 0.936 - SJR, Q1 - SJR, karentované - CCC). Dostupné na: <https://doi.org/10.1016/j.ceramint.2020.09.283>

## Programy: DoktoGranty

### 27.) Corrosion of Superalloys in Energy Application (*Corrosion of Superalloys in Energy Application*)

<b>Zodpovedný riešiteľ:</b>	Ramu Ambati
<b>Trvanie projektu:</b>	1.1.2021 / 31.12.2021
<b>Evidenčné číslo projektu:</b>	APP0156
<b>Organizácia je koordinátorom projektu:</b>	áno
<b>Koordinátor:</b>	Ústav anorganickej chémie SAV
<b>Počet spoluriešiteľských inštitúcií:</b>	0
<b>Čerpané financie:</b>	SAV: 2000 €

#### Dosiahnuté výsledky:

Bola študovaná korózna odolnosť dvoch zliatin Hastelloy®-N a Hastelloy®-G35 voči prchavým produktom, vznikajúcim pri teplote 800 °C a výdrži 48 hodín z roztavenej eutektickej zmesi LiF-NaF-KF a prostredí tvorenom zmesou argónu a 5% kyslíka. Prchavé produkty zo zmesi LiF-NaF-KF napádajú povrch skúmaných zliatin a korózneho ataku sa zúčastňuje i kyslík prostredia Ar+5%O<sub>2</sub>. Korózný atak spôsoboval nárast hmotnosti skúmaných zliatin spôsobenou tvorbou tenkých povlakov na ich povrchu. Ukázalo sa, že korózne vrstvy nie sú stabilné, odlupujú sa od povrchu zliatin. Dôvodom môžu byť rozdielne koeficienty tepelnej rozťažnosti. Mapovanie povrchu Hastelloy®-N ukázalo, že fluoridy sa tvoria v oblastiach ochudobnených o Mo a tiež sa tvorí fluorid Mo, čo naznačuje termodynamickú stabilitu týchto zlúčenín. Mapovanie Hastelloy®-G35 ukázalo vysokú koncentráciu oxidovej vrstvy bohatej na Cr.

#### Výstupy:

AMBATI, Ramu - PAVLÍK, Viliam - BOČA, Miroslav. Interaction of Hastelloy-N and Hastelloy-G35 alloys with vapours generated from molten FLiNaK salt. In ChemZi: Slovenský časopis o chémii pre chemické vzdelávanie, výskum a priemysel. Bratislava: Slovenská chemická spoločnosť, 2021, roč. 17, č. 1, s. 98-99. ISSN 1336-7242.

## Programy: Európsky fond regionálneho rozvoja (EFRR)

### 28.) Rozvoj a podpora výskumno – vývojových aktivít Centra pre testovanie kvality a diagnostiku materiálov v oblastiach špecializácie RIS3 SK (ITMS2014+: 313011W442) (*Rozvoj a podpora výskumno – vývojových aktivít Centra pre testovanie kvality a diagnostiku materiálov v oblastiach špecializácie RIS3*)

SK)

<b>Zodpovedný riešiteľ:</b>	Dušan Galusek
<b>Trvanie projektu:</b>	1.1.2019 / 30.6.2023
<b>Evidenčné číslo projektu:</b>	ITMS2014+ 313011W442
<b>Organizácia je koordinátorom projektu:</b>	nie
<b>Koordinátor:</b>	Trenčianska univerzita Alexandra Dubčeka v Trenčíne
<b>Počet spoluriešiteľských inštitúcií:</b>	4 - Slovensko: 4
<b>Čerpané financie:</b>	ŠF: 99581 €

Dosiahnuté výsledky:

**Príloha C****Publikačná činnosť organizácie (generovaná z ARL)****ABC Kapitoly vo vedeckých monografiách vydané v zahraničných vydavateľstvách**

- ABC01 GALUSKOVÁ, Dagmar - GALUSEK, Dušan. Corrosion and degradation of glass. In Encyclopedia of Materials: Technical ceramics and glasses. - Oxford : Elsevier, 2021, 2021, vol. 1, p. 932-940. ISBN 978-0-12-818542-1. Dostupné na internete: <http://dx.doi.org/10.1016/B978-0-12-818542-1.00069-2>
- ABC02 TATARKOVÁ, Monika - TATARKO, Peter - ŠAJGALÍK, Pavol. Si<sub>3</sub>N<sub>4</sub> ceramics, structure and properties. In Encyclopedia of Materials: Technical ceramics and glasses. - Oxford : Elsevier, 2021, 2021, vol. 2, p. 109-118. ISBN 978-0-12-818542-1. Dostupné na: <https://doi.org/10.1016/B978-0-12-818542-1.00021-7>

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- ADCA01 AKUSEVICH, A. - PARCHOVIANSKÁ, I. - PARCHOVIANSKÝ, Milan - PRNOVÁ, Anna - LOFAJ, František - VOJTKO, Marek - KLEMENT, Róbert\*\*. Glass-ceramic Ce<sup>3+</sup>-doped YAG-Al<sub>2</sub>O<sub>3</sub> composites prepared by sintering of glass microspheres. In International Journal of Applied Glass Science, 2021, vol. 12, no. 4, p. 497-508. (2020: 2.029 - IF, Q2 - JCR, 0.383 - SJR, Q3 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 2041-1286. Dostupné na: <https://doi.org/10.1111/ijag.16174>
- ADCA02 AMSLER, Jonas\*\* - PLESSOW, Philipp N. - STUDDT, Felix - BUČKO, Tomáš\*\*. Anharmonic correction to adsorption free energy from DFT-based MD using thermodynamic integration. In Journal of Chemical Theory and Computation, 2021, vol. 17, no. 2, p. 1155-1169. (2020: 6.006 - IF, Q1 - JCR, 2.001 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 1549-9618. Dostupné na: <https://doi.org/10.1021/acs.jctc.0c01022>
- ADCA03 BAČÍK, Peter\*\* - FRIDRICHOVÁ, Jana - UHER, Pavel - VACULOVIČ, T. - KUREKOVÁ, Valéria - ŠKODA, Radek - DEKAN, Július - MIGLIERINI, Marcel - MALÍČKOVÁ, Iveta. Beryl crystal chemistry and trace elements: Indicators of pegmatite development and fractionation (Damara Belt, Namibia). In Lithos, 2021, vol. 404-405, p. 106441-1-106441-16. (2020: 4.004 - IF, Q1 - JCR, 1.899 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 0024-4937. Dostupné na: <https://doi.org/10.1016/j.lithos.2021.106441>
- ADCA04 BARLOG, Martin\*\* - PÁLKOVÁ, Helena - BUJDÁK, Juraj. Luminescence of a laser dye in organically-modified layered silicate pigments. In Dyes and Pigments, 2021, vol. 191, p. 109380-1-109380-11. (2020: 4.889 - IF, Q1 - JCR, 0.827 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 0143-7208. Dostupné na: <https://doi.org/10.1016/j.dyepig.2021.109380>
- ADCA05 BOHÁČ, Peter\*\* - SASAI, Ryo - SOONTORNCHAIYAKUL, W. - CZÍMEROVÁ, Adriana - BUJDÁK, Juraj. Resonance energy transfer between cyanine dyes in hybrid films of layered silicate prepared by layer-by-layer method. In Applied Clay Science, 2021, vol. 202, p. 105985-1-105985-9. (2020: 5.467 - IF, Q1 - JCR, 1.062 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 0169-1317. Dostupné na: <https://doi.org/10.1016/j.clay.2021.105985>
- ADCA06 BOJE, Astrid - TAIFAN, William E. - STRÖM, Henrik - BUČKO, Tomáš - BALTRUSAITIS, Jonas - HELLMAN, Anders\*\*. First-principles-informed energy span and microkinetic analysis of ethanol catalytic conversion to 1,3-butadiene on MgO. In Catalysis Science and Technology, 2021, vol. 11, no. 20, p. 6682-6693. (2020: 6.119 - IF, Q2 - JCR, 1.635 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 2044-4753. Dostupné na: <https://doi.org/10.1039/d1cy00419k>
- ADCA07 CASIER, Bastien - CHAGAS DA SILVA, Mauricio - BADAWI, Michael - PASCALE, Fabien - BUČKO, Tomáš - LEBÈGUE, Sébastien - ROCCA, Dario\*\*. Hybrid localized graph kernel for machine learning energy-related properties of molecules and solids. In Journal of Computational Chemistry, 2021, vol. 42, no. 20, p. 1390-1401. (2020: 3.376 - IF, Q2 - JCR, 0.907 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 0192-8651. Dostupné na: <https://doi.org/10.1002/jcc.26550>
- ADCA08 DADI, Nitin Chandra teja - DOHÁL, Matúš - MEDVECKÁ, Veronika - BUJDÁK, Juraj - KOČI,

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- ADCA09 DADI, Nitin Chandra teja - BUJDÁK, Juraj\*\* - MEDVECKÁ, Veronika - PÁLKOVÁ, Helena - BARLOG, Martin - BUJDÁKOVÁ, Helena\*\*. Surface characterization and anti-biofilm effectiveness of hybrid films of polyurethane functionalized with saponite and phloxine B. In *Materials*, 2021, vol. 14, no. 14, p. 7583-1-7583-21. (2020: 3.623 - IF, Q1 - JCR, 0.682 - SJR, Q2 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 1996-1944. Dostupné na: <https://doi.org/10.3390/ma14247583>
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- ADCA12 DASAN, Arish\*\* - TALIMIAN, Ali - KRAXNER, Jozef - GALUSEK, Dušan - ELSAYED, Hamada - BERNARDO, Enrico\*\*. Akermanite glass microspheres: Preparation and perspectives of sinter-crystallization. In *International Journal of Applied Glass Science*, 2021, vol. 12, no. 4, p. 551-561. (2020: 2.029 - IF, Q2 - JCR, 0.383 - SJR, Q3 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 2041-1286. Dostupné na: <https://doi.org/10.1111/ijag.16115>
- ADCA13 DENG, Qiang - SLANÝ, Michal\*\* - ZHANG, Huani - GU, Xuefan - LI, Yongfei - DU, Weichao - CHEN, Gang. Synthesis of alkyl aliphatic hydrazine and application in crude oil as flow improvers. In *Energies*, 2021, vol. 14, no. 15, p. 4703-1-4703-11. (2020: 3.004 - IF, Q3 - JCR, 0.598 - SJR, Q2 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 1996-1073. Dostupné na: <https://doi.org/10.3390/en14154703>
- ADCA14 DESMARAIS, Jacques K.\*\* - KOMOROVSKÝ, Stanislav - FLAMENT, Jean-Pierre - ERBA, Alessandro. Spin-orbit coupling from a two-component self-consistent approach. II. Non-collinear density functional theories. In *Journal of Chemical Physics*, 2021, vol. 154, no. 20, p. 204110-1-204110-15. (2020: 3.488 - IF, Q1 - JCR, 1.071 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 0021-9606. Dostupné na: <https://doi.org/10.1063/5.0051447>
- ADCA15 DOGRUL, Fulden - OŽÓG, Paulina - MICHÁLEK, Martin - ELSAYED, Hamada - GALUSEK, Dušan - LIVERANI, Liliana - BOCCACCINI, Aldo - BERNARDO, Enrico\*\*. Polymer-derived biosilicate (R)-like glass-ceramics: Engineering of formulations and additive manufacturing of three-dimensional scaffolds. In *Materials*, 2021, vol. 14, no. 18, p. 5170-1-5170-16. (2020: 3.623 - IF, Q1 - JCR, 0.682 - SJR, Q2 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 1996-1944. Dostupné na: <https://doi.org/10.3390/ma14185170>
- ADCA16 DUSZA, Ján - CSANÁDI, Tamás\*\* - MEDVEĎ, Dávid - SEDLÁK, Richard - VOJTKO, Marek - IVOR, Michal - ÜNSAL, Hakan - TATARKO, Peter - TATARKOVÁ, Monika - ŠAJGALÍK, Pavol. Nanoindentation and tribology of a (Hf-Ta-Zr-Nb-Ti)C high-entropy carbide. In *Journal of the European Ceramic Society*, 2021, vol. 41, no. 11, p. 5417-5426. (2020: 5.302 - IF, Q1 - JCR, 1.204 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 0955-2219. Dostupné na: <https://doi.org/10.1016/j.jeurceramsoc.2021.05.002>
- ADCA17 ELSAYED, Hamada - RABELO MONICH, Patricia - SAVIO, Gianpaolo - HARTMANN, Malte - BOCCACCINI, Aldo - GALUSEK, Dušan - KRAXNER, Jozef - BERNARDO, Enrico\*\*. Alkali-free processing of advanced open-celled sinter-crystallized glass-ceramics. In *International Journal of Applied Glass Science*, 2021, vol. 12, no. 4, p. 531-540. (2020: 2.029 - IF, Q2 - JCR, 0.383 - SJR, Q3 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 2041-1286. Dostupné na: <https://doi.org/10.1111/ijag.16106>
- ADCA18 FURKA, S. - FURKA, D. - DADI, Nitin Chandra teja - PALACKA, Patrik - HROMNÍKOVÁ, Dominika - SANTANA, Julio Ariel Duenas - PINEDA, Javier Díaz - CASAS, Saul Duenas - BUJDÁK, Juraj. Novel antimicrobial materials designed for the 3D-printing of medical devices

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- ADCA19 GALUSKOVÁ, Dagmar\*\* - KAŇKOVÁ, Hana - ŠVANČÁRKOVÁ, Anna - GALUSEK, Dušan. Early-stage dissolution kinetics of silicate-based bioactive glass under dynamic conditions: Critical evaluation. In Materials, 2021, vol. 14, no. 12, p. 3384-1-3384-17. (2020: 3.623 - IF, Q1 - JCR, 0.682 - SJR, Q2 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 1996-1944. Dostupné na: <https://doi.org/10.3390/ma14123384>
- ADCA20 GEŠVANDTNEROVÁ, Monika\*\* - ROCCA, Dario - BUČKO, Tomáš\*\*. Methanol carbonylation over acid mordenite: Insights from ab initio molecular dynamics and machine learning thermodynamic perturbation theory. In Journal of Catalysis, 2021, vol. 396, p. 166-178. (2020: 7.920 - IF, Q1 - JCR, 2.337 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 0021-9517. Dostupné na: <https://doi.org/10.1016/j.jcat.2021.02.011>
- ADCA21 GRIEBENOW, Kristin\*\* - MUNOZ, Francisco - TAGIARA, Nagia S. - KLEMENT, Róbert - PRNOVÁ, Anna - WOLFRUM, Bruno - KAMITSOS, Efstratios I. - DURAN, Alicia - GALUSEK, Dušan. Structure and fluorescence properties of Dy-doped alkaline-earth borophosphate glasses. In International Journal of Applied Glass Science, 2021, vol. 12, no. 4, p. 472-484. (2020: 2.029 - IF, Q2 - JCR, 0.383 - SJR, Q3 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 2041-1286. Dostupné na: <https://doi.org/10.1111/ijag.16105>
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- ADCA23 HANZEL, Ondřej\*\* - LENČEŠ, Zoltán - TATARKO, Peter - SEDLÁK, Richard - DLOUHÝ, Ivo - DUSZA, Ján - ŠAJGALÍK, Pavol. Preparation and properties of layered SiC-graphene composites for EDM. In Materials, 2021, vol. 14, no. 11, p. 2916-1-2916-14. (2020: 3.623 - IF, Q1 - JCR, 0.682 - SJR, Q2 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 1996-1944. Dostupné na: <https://doi.org/10.3390/ma14112916>
- ADCA24 HRUŠKA, Branislav\*\* - NOWICKA, Aleksandra - CHROMČÍKOVÁ, Mária - GREINER-WRONA, Elżbieta - SMOLÍK, Jan - SOLTÉZS, Vojtech - LIŠKA, Marek. Raman spectroscopic study of corroded historical glass. In International Journal of Applied Glass Science, 2021, vol. 12, no. 4, p. 613-620. (2020: 2.029 - IF, Q2 - JCR, 0.383 - SJR, Q3 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 2041-1286. Dostupné na: <https://doi.org/10.1111/ijag.16010>
- ADCA25 HUJOVÁ, Miroslava\*\* - RABELO MONICH, Patricia - KAŇKOVÁ, Hana - LUCAS, Hugo - XAKALASHE, Buhle - FRIEDRICH, Bernd - KRAXNER, Jozef - GALUSEK, Dušan - BERNARDO, Enrico. New glass-based binders from engineered mixtures of inorganic waste. In International Journal of Applied Glass Science, 2021, vol. 12, no. 4, p. 570-580. (2020: 2.029 - IF, Q2 - JCR, 0.383 - SJR, Q3 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 2041-1286. Dostupné na: <https://doi.org/10.1111/ijag.16262>
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- ADCA27 CHROMČÍKOVÁ, Mária\*\* - HRUŠKA, Branislav - SVOBODA, Roman - LIŠKA, Marek - NOWICKA, Aleksandra - BRUNEEL, E. - DE BUYSSER, Klaartje. Identification of surface active components in glass forming melts by thermodynamic model. In Journal of Non-Crystalline Solids, 2021, vol. 551, p. 120415-1-120415-7. (2020: 3.531 - IF, Q1 - JCR, 0.764 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 0022-3093. Dostupné na: <https://doi.org/10.1016/j.jnoncrysol.2020.120415>
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- ADCA31 KITYK, A.\*\* - HNATKO, Miroslav - PAVLÍK, Viliam - BOČA, Miroslav. Electrochemical surface treatment of manganese stainless steel using several types of deep eutectic solvents. In Materials Research Bulletin, 2021, vol. 141, p. 111348-1-111348-11. (2020: 4.641 - IF, Q2 - JCR, 0.861 - SJR, Q1 - SJR, karentované - CCC). (2021 - Current Contents). ISSN 0025-5408. Dostupné na: <https://doi.org/10.1016/j.materresbull.2021.111348>
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3. [1.1] PHAVONGKHAM, V. - WATTANASIRIWECH, S. - CHENG, T. W. - WATTANASIRIWECH, D. Effects of surfactant on thermo-mechanical behavior of geopolymer foam paste made with sodium perborate foaming agent. In *CONSTRUCTION AND BUILDING MATERIALS. ISSN 0950-0618*, 2020, vol. 243, art. no. 118282., Registrované v: WOS
4. [1.1] RANJBAR, N. - KASHEFI, A. - YE, G. - MEHRALI, M. Effects of heat and pressure on hot-pressed geopolymer. In *CONSTRUCTION AND BUILDING MATERIALS. ISSN 0950-0618*, 2020, vol. 231, art. no. 117106., Registrované v: WOS

#### ADEB Vedecké práce v ostatných zahraničných časopisoch – neimpaktovaných

ADEB01 GALUSKOVÁ, Dagmar - ŠAJGALÍK, Pavol - GALUSEK, Dušan - HNATKO, Miroslav. Corrosion of alumina ceramics in an aqueous solution of sodium chloride. In *Key Engineering Materials*, 2009, vol. 413, p. 283-286. (2008: 0.192 - SJR, Q3 - SJR). (2009 - SCOPUS). ISSN 1013-9826. Dostupné na: <https://doi.org/10.4028/www.scientific.net/KEM.409.283>

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1. [1.1] MOGALE, Ntebogeng F. - MATIZAMHUKA, Wallace R. A Study on the Effect of Ultrafine SiC Additions on Corrosion and Wear Performance of Alumina-Silicon Carbide Composite Material Produced by SPS Sintering. In *METALS*, 2020, vol. 10, no. 10, pp., Registrované v: WOS

ADEB02 KARELL, Radovan - CHROMČÍKOVÁ, Mária - LIŠKA, Marek. Structure and properties of selected zirconia silicate glasses. In *Advanced Materials Research. - Zurich : Trans. Tech. Publ.*, 2008, vol. 39-40, p. 173-176. (2007: 0.180 - SJR, Q3 - SJR). ISSN 1022-6680. Dostupné na: <https://doi.org/10.4028/www.scientific.net/amr.39-40.173>

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1. [1.1] MUELLER, Dirk - HESS, Kai-Uwe - KUEPPERS, Ulrich - DINGWELL, Donald B. Effects of the dissolution of thermal barrier coating materials on the viscosity of remelted volcanic ash. In *AMERICAN MINERALOGIST. ISSN 0003-004X*, 2020, vol. 105, no. 7, pp. 1104-1107. Dostupné na: <https://doi.org/10.2138/am-2020-7334>, Registrované v: WOS

ADEB03 KAUPP, Martin - MALKIN, Vladimír - MALKINA, Oľga - SALAHUB, Dennis R. Ab initio ECP/DFT calculation and interpretation of carbon and oxygen NMR chemical shift tensors in transition-metal

carbonyl complexes. In Chemistry -A European Journal, 1996, vol. 2, no. 1, p. 24-30. ISSN 0947-6539. Dostupné na: <https://doi.org/10.1002/chem.19960020108>

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ADEB04 LIČKO, T. - ŠAJGALÍK, Pavol. Preparation of alpha-Si<sub>3</sub>N<sub>4</sub> powder and ceramics reinforced by beta-Si<sub>3</sub>N<sub>4</sub> whiskers. In Ceramics-Silikáty, 1991, vol. 35, no. 2, p. 127-. ISSN 0862-5468.

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1. [1.1] USKOKOVIC, Vuk. Earthlike and Its Discontents: A Historical Critical Review of Iron (Oxide) Particles Singly and Doubly Shelled with Silica and/or Carbon. In ACS EARTH AND SPACE CHEMISTRY. ISSN 2472-3452, 2020, vol. 4, no. 10, pp. 1843-1877. Dostupné na: <https://doi.org/10.1021/acsearthspacechem.0c00173>., Registrované v: WOS

ADEB05 MALKIN, Vladimír - MALKINA, Oľga - STEINEBRUNNER, G. - HUBER, H. Solvent effect on the NMR chemical shieldings in water calculated by a combination of molecular dynamics and density functional theory. In Chemistry - A European Journal, 1996, vol. 2, no. 4, p. 452-457. ISSN 0947-6539. Dostupné na: <https://doi.org/10.1002/chem.19960020415>

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1. [1.1] JIANG, Jingjing - JIN, Mingjie - LI, Xiaoyi - MENG, Qin - NIU, Jian - LONG, Xuwei. Recent progress and trends in the analysis and identification of rhamnolipids. In APPLIED MICROBIOLOGY AND BIOTECHNOLOGY. ISSN 0175-7598, 2020, vol. 104, no. 19, pp. 8171-8186. Dostupné na: <https://doi.org/10.1007/s00253-020-10841-3>., Registrované v: WOS
2. [1.1] REIMANN, Marc - KAUPP, Martin. Evaluation of an Efficient 3D-RISM-SCF Implementation as a Tool for Computational Spectroscopy in Solution. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2020, vol. 124, no. 37, pp. 7439-7452. Dostupné na: <https://doi.org/10.1021/acs.jpca.0c06322>., Registrované v: WOS

ADEB06 TATARKO, Peter - LOJANOVÁ, Š. - DUSZA, Ján - ŠAJGALÍK, Pavol. Characterization of rare-earth doped Si<sub>3</sub>N<sub>4</sub>/SiC micro/nano-composites. In Processing and Application of Ceramics, 2010, vol. 4, no. 1, p. 25-32.

Citácie:

1. [1.1] NERSISYAN, Hayk - HUYNH THANH NAM - RI, Vladislav - WOO, Hwa Young - HONG, Soon-Jik - LEE, Jong Hyeon. 3D self-assemblies of beta-Si<sub>3</sub>N<sub>4</sub>: Synthesis, characterization and growth mechanism. In JOURNAL OF CRYSTAL GROWTH. ISSN 0022-0248, 2020, vol. 549, no., pp., Registrované v: WOS

ADEB07 TATARKO, Peter - LOJANOVÁ, Š. - CHLUP, Zdeněk - DUSZA, Ján - ŠAJGALÍK, Pavol. Microstructure and mechanical properties of rare-earth doped Si<sub>3</sub>N<sub>4</sub> and Si<sub>3</sub>N<sub>4</sub>/SiC ceramics. In Advances in Science and Technology, 2010, vol. 65, p. 78-85. ISSN 2299-8624.

Citácie:

1. [1.1] YE, C. C. - RU, H. Q. - QIN, Z. B. - ZHAO, S. W. - JIA, H. S. - CHEN, D. L. Silicon nitride composites with magnesia and alumina additives: Toughening mechanisms and mechanical properties. In MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING. ISSN 0921-5093, 2020, vol. 779, no., pp., Registrované v: WOS

#### ADFB Vedecké práce v ostatných domácich časopisoch – neimpaktovaných

ADFB01 ZEMANOVÁ, Matilda - LOKAJ, Ján - KARLOVÁ, Mária - MADEJOVÁ, Jana. Influence of pre-treatment on zirconium based conversion coating on AA2024. In Acta Chimica Slovaca, 2017, vol. 10, no. 2, p. 101-106. ISSN 1337-978X. Dostupné na: <https://doi.org/10.1515/acs-2017-0018>

Citácie:

1. [1.1] MOFIDABADI, Amir Hossein Jafari - BAHLAKEH, Ghasem - RAMEZANZADEH, Bahram. Explorations of the adhesion and anti-corrosion properties of the epoxy coating on the carbon steel surface modified by Eu<sub>2</sub>O<sub>3</sub> nanostructured film. In JOURNAL OF MOLECULAR LIQUIDS. ISSN 0167-7322, 2020, vol. 314, no., pp., Registrované v: WOS

#### ADMA Vedecké práce v zahraničných impaktovaných časopisoch registrovaných v databázach Web of Science alebo SCOPUS

ADMA01 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, p. 324-331. (2016: 0.572 - IF, Q4 - JCR, 0.194 - SJR, Q4 - SJR). ISSN 0021-9037. Dostupné na: <https://doi.org/10.1007/s10812-017-0471-x>

Citácie:

1. [1.1] CHUCHINA, Victoria - GUBAL, Anna - LYALKIN, Yegor - GLUMOV, Oleg - TREFILOV, Ivan -



SOROKINA, Angelina - SAVINOV, Sergey - SOLOVYEV, Nikolay - GANEEV, Alexander. A study of matrix and admixture elements in fluorine-rich ionic conductors by pulsed glow discharge mass spectrometry. In *RAPID COMMUNICATIONS IN MASS SPECTROMETRY*. ISSN 0951-4198, 2020, vol. 34, no. 11, pp. Dostupné na: <https://doi.org/10.1002/rcm.8786>, Registrované v: WOS

2. [1.1] SITUM, Arthur - BEAM, Jeremiah C. - HUGHES, Kebbi A. - ROWSON, John - CRAWFORD, Andrew - GROSVENOR, Andrew P. Analysis of low concentration U species within U mill tailings using X-ray microprobe. In *JOURNAL OF ELECTRON SPECTROSCOPY AND RELATED PHENOMENA*. ISSN 0368-2048, 2020, vol. 244, no., pp. Dostupné na: <https://doi.org/10.1016/j.elspec.2020.146992>, Registrované v: WOS

ADMA02 KORENKO, Michal - VASKOVÁ, Zuzana - ŠIMKO, František - ŠIMURDA, Michal - AMBROVÁ, Marta - SHI, Zhong-ning. Electrical conductivity and viscosity of cryolite electrolytes for solar grade silicon (Si-SoG) electrowinning. In *Transactions of Nonferrous Metals Society of China*, 2014, vol. 24, no. 12, p. 3944-3948. (2013: 1.001 - IF, Q2 - JCR, 0.834 - SJR). ISSN 1003-6326. Dostupné na: [https://doi.org/10.1016/S1003-6326\(14\)63554-8](https://doi.org/10.1016/S1003-6326(14)63554-8)

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1. [1.1] PADAMATA, Sai Krishna - YASINSKIY, Andrey S. - POLYAKOV, Petr. Anodic process on Cu?Al alloy in KF?AlF 3?Al 2 O 3 melts and suspensions. In *TRANSACTIONS OF NONFERROUS METALS SOCIETY OF CHINA*. ISSN 1003-6326, 2020, vol. 30, no. 5, pp. 1419-1428., Registrované v: WOS

ADMA03 LIU, Aimin - SHI, Zhongning - XIE, K. - HU, Xianwei - GAO, Bingliang - KORENKO, Michal - WANG, Zhaowen. Extraction of Al-Si master alloy and alumina from coal fly ash. In *Journal of Mining and Metallurgy : Section B: Metallurgy*, 2017, vol. 53, no. 2, p. 155-162. (2016: 0.804 - IF, Q3 - JCR, 0.529 - SJR, Q2 - SJR). ISSN 1450-5339. Dostupné na: <https://doi.org/10.2298/JMMB160616006L>

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1. [1.1] JU, Tongyao - JIANG, Jianguo - MENG, Yuan - YAN, Feng - XU, Yiwen - GAO, Yuchen - AIHEMAITI, Aikelaimu. An investigation of the effect of ultrasonic waves on the efficiency of silicon extraction from coal fly ash. In *ULTRASONICS SONOCHEMISTRY*. ISSN 1350-4177, 2020, vol. 60, no., pp. Dostupné na: <https://doi.org/10.1016/j.ultsonch.2019.104765>, Registrované v: WOS

2. [1.1] SHI, Yuan - JIANG, Kai-xi - ZHANG, Ting-an - LV, Guo-zhi. Cleaner alumina production from coal fly ash: Membrane electrolysis designed for sulfuric acid leachate. In *JOURNAL OF CLEANER PRODUCTION*. ISSN 0959-6526, 2020, vol. 243, no., pp. Dostupné na: <https://doi.org/10.1016/j.jclepro.2019.118470>, Registrované v: WOS

3. [1.1] SHI, Yuan - JIANG, Kai-xi - ZHANG, Ting-an. Cleaner extraction of alumina from coal fly ash: Baking-electrolysis method. In *FUEL*. ISSN 0016-2361, 2020, vol. 273, no., pp. Dostupné na: <https://doi.org/10.1016/j.fuel.2020.117697>, Registrované v: WOS

ADMA04 PATEL, Niketan Sarabhai\*\* - PAVLÍK, Viliam - KUBÍKOVÁ, Blanka - NOSKO, Martin - DANIELIK, Vladimír - BOČA, Miroslav. Corrosion behaviour of Ni-based superalloys in molten FLiNaK salts. In *Corrosion Engineering, Science and Technology*, 2019, vol. 54, no. 1, p. 46-53. (2018: 1.393 - IF, Q2 - JCR, 0.387 - SJR, Q2 - SJR). ISSN 1478-422X. Dostupné na: <https://doi.org/10.1080/1478422X.2018.1525829>

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1. [1.1] JIANG, Li - WANG, Wei - YE, Xiang-Xi - LI, Chao-Wen - LIANG, Jian-Ping - WANG, De-Jun - LI, Zhi-Jun. Unexpected effect of hydroxyl radical on tellurium corrosion of the Ni-Mo-Cr-Nb based alloy. In *CORROSION SCIENCE*. ISSN 0010-938X, 2020, vol. 173, no., pp. Dostupné na: <https://doi.org/10.1016/j.corsci.2020.108748>, Registrované v: WOS

2. [1.1] RONNE, Arthur - HE, Lingfeng - DOLZHIKOV, Dmitriy - XIE, Yi - GE, Mingyuan - HALSTENBERG, Phillip - WANG, Yachun - MANARD, Benjamin T. - XIAO, Xianghui - LEE, Wah-Keat - SASAKI, Kotaro - DAI, Sheng - MAHURIN, Shannon M. - CHEN-WIEGART, Yu-Chen Karen. Revealing 3D Morphological and Chemical Evolution Mechanisms of Metals in Molten Salt by Multimodal Microscopy. In *ACS APPLIED MATERIALS & INTERFACES*. ISSN 1944-8244, 2020, vol. 12, no. 15, pp. 17321-17333. Dostupné na: <https://doi.org/10.1021/acsami.9b19099>, Registrované v: WOS

3. [1.1] ZHAO, Y. - ZHAO, C. Y. - MARKIDES, C. N. - WANG, H. - LI, W. Medium- and high-temperature latent and thermochemical heat storage using metals and metallic compounds as heat storage media: A technical review. In *APPLIED ENERGY*. ISSN 0306-2619, 2020, vol. 280, no., pp. Dostupné na: <https://doi.org/10.1016/j.apenergy.2020.115950>, Registrované v: WOS

ADMA05 SILNÝ, A. - KORENKO, Michal - DANĚK, V. - CHRENKOVÁ, Marta. Carbon consumption during laboratory aluminum electrolysis. In *Canadian Metallurgical Quarterly*, 2006, vol. 45, no. 3, p. 275-281. (2005: 0.265 - IF, Q3 - JCR, 0.368 - SJR, Q1 - SJR). ISSN 0008-4433. Dostupné na: <https://doi.org/10.1179/cmqr.2006.45.3.275>

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1. [1.1] STANIC, Nikolina - BO, Embla Tharaldsen - SANDNES, Espen. CO and CO2 Anode Gas Concentration at Lower Current Densities in Cryolite Melt. In *METALS*, 2020, vol. 10, no. 12, pp. Dostupné na: <https://doi.org/10.3390/met10121694>, Registrované v: WOS

ADMA06 SINGH, Meinam Annebushan\*\* - RAJBONGSHI, Sanjib Kr - SARMA, Deba Kumar - HANZEL,



Ondrej - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Surface and porous recast layer analysis in  $\mu$ -EDM of MWCNT-Al<sub>2</sub>O<sub>3</sub> composites. In *Materials and Manufacturing Processes*, 2019, vol. 34, no. 5, p. 567-579. (2018: 3.350 - IF, Q2 - JCR, 1.111 - SJR, Q1 - SJR). ISSN 1042-6914. Dostupné na: <https://doi.org/10.1080/10426914.2019.1566617>

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1. [1.1] MING, Wuyi - JIA, Haojie - ZHANG, Hongmei - ZHANG, Zhen - LIU, Kun - DU, Jinguang - SHEN, Fan - ZHANG, Guojun. A comprehensive review of electric discharge machining of advanced ceramics. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2020, vol. 46, no. 14, pp. 21813-21838. Dostupné na: <https://doi.org/10.1016/j.ceramint.2020.05.207>., Registrované v: WOS
2. [1.1] SINGH, Ramver - DVIVEDI, Akshay - KUMAR, Pradeep. EDM of high aspect ratio micro-holes on Ti-6Al-4V alloy by synchronizing energy interactions. In *MATERIALS AND MANUFACTURING PROCESSES*. ISSN 1042-6914, 2020, vol. 35, no. 11, pp. 1188-1203. Dostupné na: <https://doi.org/10.1080/10426914.2020.1762207>., Registrované v: WOS
3. [1.1] ZENG, Liang - MA, Chunyang - ZUO, Hanrui - XIA, Fafeng - LI, Qiang. PULSE ELECTRODEPOSITED NANO-SIZED Ni-AlN THIN FILMS: PREPARATION AND CORROSION RESISTANCE PREDICTION USING BACKWARD PROPAGATION NETWORK MODEL. In *SURFACE REVIEW AND LETTERS*. ISSN 0218-625X, 2020, vol. 27, no. 10, pp. Dostupné na: <https://doi.org/10.1142/S0218625X19502238>., Registrované v: WOS

ADMA07 SINGH, Meinam Annebushan\*\* - SARMA, Deba Kumar - HANZEL, Ondrej - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Surface characteristics and erosion phenomena in WEDM of alumina composites. In *Materials and Manufacturing Processes*, 2018, vol. 33, no. 16, p. 1815-1821. (2017: 2.669 - IF, Q2 - JCR, 0.948 - SJR, Q1 - SJR). ISSN 1042-6914. Dostupné na: <https://doi.org/10.1080/10426914.2018.1512127>

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1. [1.1] GRIGORIEV, Sergey N. - VOLOSOVA, Marina A. - OKUNKOVA, Anna A. - FEDOROV, Sergey V. - HAMDY, Khaled - PODRABINNIK, Pavel A. - PIVKIN, Petr M. - KOZUCHKIN, Mikhail P. - PORVATOV, Artur N. Wire Tool Electrode Behavior and Wear under Discharge Pulses. In *TECHNOLOGIES*, 2020, vol. 8, no. 3, pp. Dostupné na: <https://doi.org/10.3390/technologies8030049>., Registrované v: WOS
2. [1.1] MANDAL, Kingshuk - BOSE, Dipankar - MITRA, Souren - SARKAR, Soumya. Experimental investigation of process parameters in WEDM of Al 7075 alloy. In *MANUFACTURING REVIEW*. ISSN 2265-4224, 2020, vol. 7, no., pp. Dostupné na: <https://doi.org/10.1051/mfreview/2020021>., Registrované v: WOS

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

ADMB01 KAŠIAROVÁ, Monika - PRAMUKOVÁ, Zuzana - BODIŠOVÁ, Katarína - DOMANICKÁ, Magdaléna - HNATKO, Miroslav - DUSZA, Ján - ŠAJGALÍK, Pavol - GROMOŠOVÁ, Silvia. Mechanical properties of porous Si<sub>3</sub>N<sub>4</sub> ceramics. In *Key Engineering Materials*, 2014, vol. 586, p. 166-169. (2013: 0.190 - SJR). (2014 - SCOPUS). ISSN 1013-9826. Dostupné na: <https://doi.org/10.4028/www.scientific.net/KEM.586.166> (Local mechanical properties 2012 : LMP 2012)

Citácie:

1. [1.1] MIEDZINSKA, Danuta. Influence of Grains Shape Irregularity in Porous Ceramics-Numerical Study. In *MATERIALS*, 2020, vol. 13, no. 8, pp., Registrované v: WOS

ADMB02 KOMADEL, Peter - MADEJOVÁ, Jana - VALÚCHOVÁ, Jana - JANEK, Marián - BUJDÁK, Juraj. Fixation of Li<sup>+</sup> 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] HE, Qiuzhi - ZHU, Runliang - CHEN, Qingze - ZHU, Yanping - YANG, Yixuan - DU, Jing - ZHU, Jianxi - HE, Hongping. One-pot synthesis of the reduced-charge montmorillonite via molten salts treatment. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2020, vol. 186, no., pp. Dostupné na: <https://doi.org/10.1016/j.clay.2019.105429>., Registrované v: WOS

ADMB03 PÁLKOVÁ, Helena - MADEJOVÁ, Jana. FTIR study of structural modifications of Li-montmorillonites. In *Solid State Phenomena*, 2003, vol.90-91, p. 503-508. (2003 - Current Contents). ISSN 1012-0394. Dostupné na: <https://doi.org/10.4028/www.scientific.net/ssp.90-91.503> (Solid State Chemistry V : 5th International Conference on Solid State Chemistry)

Citácie:

1. [1.1] AMAYA, Jahaziel - BOBADILLA, Luis - AZANCOT, Lola - CENTENO, Miguel - MORENO, Sonia - MOLINA, Rafael. Modulation of the acidity of a vermiculite and its potential use as a catalytic support. In *JOURNAL OF MATERIALS SCIENCE*. ISSN 0022-2461, 2020, vol. 55, no. 15, pp. 6482-6501. Dostupné na: <https://doi.org/10.1007/s10853-020-04445-5>., Registrované v: WOS

**ADNB Vedecké práce v domácich neimpaktovaných časopisoch registrovaných v databázach Web of Science alebo SCOPUS**

ADNB01      BUJDÁK, Juraj - SLOSIARIKOVÁ, Hana - NOVÁKOVÁ, L. - ČÍČEL, Blahoslav. Fixation of lithium cations in montmorillonite. In Chemical Papers, 1991, vol. 45, no. 4, p. 499-507. ISSN 0366-6352.

Citácie:

1. [1.1] WEI, Yingchun - HE, Wenbo - QIN, Guohong - FAN, Maohong - CAO, Daiyong. Lithium Enrichment in the No. 2(1)Coal of the Hebi No. 6 Mine, Anhe Coalfield, Henan Province, China. In MINERALS, 2020, vol. 10, no. 6, pp. Dostupné na: <https://doi.org/10.3390/min10060521>., Registrované v: WOS

**AFD Publikované príspevky na domácich vedeckých konferenciách**

AFD01      MAJEROVÁ, Melinda - PRNOVÁ, Anna - ŠKRÁTEK, Martin - KLEMENT, R. - MICHÁLKOVÁ, Monika - GALUSEK, Dušan - BRUNEEL, E. - VAN DRIESSCHE, I. Magnetic properties of yttrium iron garnet polycrystalline material prepared by spray-drying synthesis. In MEASUREMENT 2015 : 10th International Conference on Measurement. Editors J. Maňka, M. Tyšler, V. Witkovský, I. Frollo. - Bratislava : Institute of Measurement Science, SAS, 2015, p. 285-288. ISBN 978-80-969672-9-2.

Citácie:

1. [1.1] GOLDWIN, J. - ARAVINTHAN, K. - RAJ, S. G. - KUMAR, R. Synthesis and characterization of nanocrystalline yttrium iron garnet ( $Y_3Fe_5O_{12}$ ) for magnetoelectric applications. In DIGEST JOURNAL OF NANOMATERIALS AND BIOSTRUCTURES. ISSN 1842-3582, 2019, vol. 14, no. 3, p. 721-725., Registrované v: WOS

2. [1.1] SAKER, K. - BOUCHEMAT, T. - LAHOUBI, M. - BOUCHEMAT, M. Enhancement of magneto-optical properties in magnetic photonic crystal slab waveguide based on yttrium iron garnet. In APPLIED NANOTECHNOLOGY AND NANOSCIENCE INTERNATIONAL CONFERENCE (ANNIC 2018). ISSN 1742-6588, 2019, vol. 1310., Registrované v: WOS

## ***Príloha D***

### **Údaje o pedagogickej činnosti organizácie**

#### Semestrálne prednášky:

doc. Ing. Miroslav Boča, DrSc.

Názov semestr. predmetu: Spectral Methods

Počet hodín za semester: 32

Názov katedry a vysokej školy: Northeastern University, Shenyang, Čína, School of Metallurgy

Ing. Blanka Kubíková, PhD.

Názov semestr. predmetu: Metódy chemického výskumu

Počet hodín za semester: 2

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

Ing. Blanka Kubíková, PhD.

Názov semestr. predmetu: Termická analýza

Počet hodín za semester: 39

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

doc. Ing. Zoltán Lenčoš, PhD.

Názov semestr. predmetu: Anorganická chémia 2

Počet hodín za semester: 8

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

doc. Ing. Zoltán Lenčoš, PhD.

Názov semestr. predmetu: Materiálová chémia

Počet hodín za semester: 4

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

Ing. Anna Prnová, PhD.

Názov semestr. predmetu: Anorganická chémia

Počet hodín za semester: 30

Názov katedry a vysokej školy: Trenčianska univerzita Alexandra Dubčeka v Trenčíne, FunGlass – Centre for Functional and Surface Functionalized Glass

#### Semestrálne cvičenia:

#### Semináre:

James Richard Asher, PhD

Názov semestr. predmetu: General Inorganic Chemistry

Počet hodín za semester: 52

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

#### Terénne cvičenia:

#### Individuálne prednášky:

**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
Česko	Peter Tatarko	5				
	Hakan Ünsal	5				
Poľsko					Helena Pálková	5
					Marek Pribus	5
					Eva Scholtzová	5
					Peter Tatarko	3
Srbsko					Ondrej Hanzel	3
					Hakan Ünsal	3
Taliansko					Miroslav Boča	4
					Blanka Kubíková	14
<b>Počet vyslaní spolu</b>	<b>2</b>	<b>10</b>			<b>8</b>	<b>42</b>

**(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
Poľsko					Małgorzata Zimowska	21
<b>Počet prijatí spolu</b>					<b>1</b>	<b>21</b>

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

Krajina	Názov konferencie	Meno pracovníka	Počet dní
Česko	Konferencia o špeciálnych anorganických pigmentoch	Anna Prnová	2
Česko (online)	NanoOstrava	Helena Pálková	4
Francúzsko (online)	NMR	Stanislav Komorovský	4
Chorvátsko	CEEC-TAC6 and Medicta2021	Mária Chromčíková	7
		Anna Prnová	7
Rusko (online)	MELTS	Miroslav Boča	7
Srbsko	CYSC	Ondrej Hanzel	2
		Peter Tatarko	2
		Hakan Ünsal	3
USA (online)	Nanomaterials and Nanotechnology	Peter Škorňa	2
	Nanomaterials and Technology	Peter Škorňa	2



<b>Spolu</b>	<b>8</b>	<b>11</b>	<b>42</b>
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Vysvetlivky: MAD - medziakademické dohody, KD - kultúrne dohody, VTS - vedecko-technická spolupráca v rámci vládnych dohôd

Skratky použité v tabuľke C:

Nanomaterials and Nanotechnology - 5th International webinar of nanomaterials and nanotechnology

CEEC-TAC6 and Medicta2021 - 6th Central and Eastern European Conference on Thermal Analysis and Calorimetry, 15th Mediterranean Conference on Calorimetry and Thermal Analysis

CYSC - Conference for Young Scientists in Ceramics

Konferencia o špeciálnych anorganických pigmentoch - 23. ročníku Konferencie o špeciálnych anorganických pigmentoch a práškových materiáloch

MELTS - Systematic research on ternary fluoride systems based on selected lanthanides. In International conference MELTS

Nanomaterials and Technology - 4th International webinar on nanomaterials and nanotechnology

NanoOstrava - , Infrared spectroscopy as powerful tool to study clay minerals subjected to various types of modification

NMR - Prediction of spectroscopic parameters for paramagnetic species containing heavy elements: Can the relativistic

DFT methods do the job? Paramagnetic NMR in f elements

**Príloha F****Vedecko-popularizačná činnosť pracovníkov organizácie SAV**

<b>Meno</b>	<b>Spoluautori</b>	<b>Typ<sup>1</sup></b>	<b>Názov</b>	<b>Miesto zverejnenia</b>	<b>Dátum alebo počet za rok</b>
doc. Ing. Miroslav Boča, DrSc.	F. Šimko, M. Korenko	TV	Magazín o vede a technológiách s Gregorom Marešom	Relácia VAT, RTVS <a href="https://www.rtvsk.sk/tel-evizia/archiv/14067/256427#445">https://www.rtvsk.sk/tel-evizia/archiv/14067/256427#445</a>	16.1.2021
Mgr. Peter Boháč, PhD.		IN	Peter Boháč: Proti chémii netreba bojovať. Chémia, ako aj celá príroda, sa riadi základnými pravidlami, ktoré treba pochopiť	EDUTECH <a href="https://www.eductech.sk/novinky/peter-bohac-proti-chemii-netreba-bojovat-chemia-ako-aj-cela-priroda-sa-riadi-zakladnymi-pravidlami-ktore-treba">https://www.eductech.sk/novinky/peter-bohac-proti-chemii-netreba-bojovat-chemia-ako-aj-cela-priroda-sa-riadi-zakladnymi-pravidlami-ktore-treba</a>	16.3.2021
Mgr. Peter Boháč, PhD.		RO	Veda na dve minúty	FUN radio <a href="https://www.funradio.sk/kategoria/veda-na-2-minuty/">https://www.funradio.sk/kategoria/veda-na-2-minuty/</a>	21.11.2021
Mgr. Stanislav Komorovský, PhD.		RO	Vedecký podcast SAV - #9 Stanislav Komorovský - Svet kvantovej mechaniky a teórie relativity	<a href="https://www.youtube.com/watch?v=wtzv2IGuamc">https://www.youtube.com/watch?v=wtzv2IGuamc</a> <a href="http://www.uach.sav.sk/sk/svet-quantovej-mechaniky-a-teorie-relativity-vedecky-podcast-sav/">http://www.uach.sav.sk/sk/svet-quantovej-mechaniky-a-teorie-relativity-vedecky-podcast-sav/</a>	8.1.2021
doc. Ing. Zoltán Lenčoš, PhD.		TV	Vedci SAV vyvíjajú nové batérie na báze sodíka	STV2 (Veda a technika)	23.1.2021
Ing. Viliam Pavlík, PhD.		IN	LETNÁ ŠKOLA MLADÝCH VEDCOV	<a href="https://www.sav.sk/?lang=sk&amp;doc=services-news&amp;source_no=20&amp;news_no=9783">https://www.sav.sk/?lang=sk&amp;doc=services-news&amp;source_no=20&amp;news_no=9783</a> , <a href="https://www.vedatechnika.sk/SK/VedaATechnikaVSR/novinky/Stranky/Letna-skola-m">https://www.vedatechnika.sk/SK/VedaATechnikaVSR/novinky/Stranky/Letna-skola-m</a>	1
Ing. Eva Scholtzová, CSc.		IN	Užitočné íly a HPC / Functional clays and HPC	Hpc focus: časopis Výpočtového strediska Slovenskej akadémie vied (dostupne <a href="https://vs.sav.sk/magazine/issues/magazine_202101_print.pdf">https://vs.sav.sk/magazine/issues/magazine_202101_print.pdf</a> )	1

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