

Ústav anorganickej chémie SAV



**Správa o činnosti organizácie SAV
za rok 2019**

Bratislava
január 2020

Obsah

1. Základné údaje o organizácii	1
2. Vedecká činnosť	3
3. Doktorandské štúdium, iná pedagogická činnosť a budovanie ľudských zdrojov pre vedu a techniku	16
4. Medzinárodná vedecká spolupráca	20
5. Koncepcia dlhodobého rozvoja organizácie	24
6. Spolupráca s univerzitami/vysokými školami a inými subjektmi v oblasti vedy a techniky, okrem aktivít uvedených v kap. 2, 3, 4.	26
7. Aplikácia výsledkov výskumu v spoločenskej a hospodárskej praxi	28
8. Aktivity pre Národnú radu SR, vládu SR, ústredné orgány štátnej správy SR a iné organizácie	29
9. Vedecko-organizačné a popularizačné aktivity	30
10. Činnosť knižnično-informačného pracoviska	36
11. Aktivity v orgánoch SAV	37
12. Hospodárenie organizácie	38
13. Nadácie a fondy pri organizácii SAV	39
14. Iné významné činnosti organizácie SAV	39
15. Vyznamenania, ocenenia a ceny udelené pracovníkom organizácie v roku 2019	39
16. Poskytovanie informácií v súlade so zákonom č. 211/2000 Z. z. o slobodnom prístupe k informáciám v znení neskorších predpisov (Zákon o slobode informácií)	40
17. Problémy a podnety pre činnosť SAV	40
 Prílohy	 42
<i>Príloha A</i> - Zoznam zamestnancov a doktorandov organizácie k 31.12.2019	42
<i>Príloha B</i> - Projekty riešené v organizácii	45
<i>Príloha C</i> - Publikačná činnosť organizácie (generovaná z ARL)	68
Ohlasy (citácie):	84
<i>Príloha D</i> - Údaje o pedagogickej činnosti organizácie	190
<i>Príloha E</i> - Medzinárodná mobilita organizácie	192
<i>Príloha F</i> - Vedecko-popularizačná činnosť pracovníkov organizácie SAV	194

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 Lenčoš, 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:

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 difraktopetriu**
Ústav merania SAV, Dúbravská cesta 9, 841 04, Bratislava 4

Vedúci organizačných zložiek a detašovaných pracovísk:

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 difraktopetriu**
doc. Ing. Miroslav Boča, DrSc.

1.2. Údaje o zamestnancoch

Tabuľka 1a Počet a štruktúra zamestnancov

Štruktúra zamestnancov	K	K		K do 35 rokov		F	P	T	O
		M	Ž	M	Ž				
Celkový počet zamestnancov	74	37	37	10	6	71	57.38	40.71	0
Vedeckí pracovníci	41	26	15	6	2	39	34.12	34.12	0
Odborní pracovníci VŠ (výskumní a vývojoví zamestnanci ¹)	9	6	3	4	1	8	6.04	5.59	0
Odborní pracovníci VŠ (ostatní zamestnanci ²)	7	3	4	0	2	7	4.28	1	0
Odborní pracovníci ÚS	13	2	11	0	1	13	10.66	0	0
Ostatní pracovníci	4	0	4	0	0	4	2.28	0	0

¹ odmeňovaní podľa 553/2003 Z.z., príloha č. 5

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

K – kmeňový stav zamestnancov v pracovnom pomere k 31.12.2019 (uvádzať zamestnancov v pracovnom pomere, vrátane riadnej materskej dovolenky, zamestnancov pôsobiacich v zahraničí, v štátnych funkciách, členov Predsedníctva SAV, zamestnancov pôsobiacich v zastupiteľských zboroch)

F – fyzický stav zamestnancov k 31.12.2019 (bez riadnej materskej dovolenky, zamestnancov pôsobiacich v zahraničí v štátnych funkciách, členov Predsedníctva SAV, zamestnancov pôsobiacich v zastupiteľských zboroch)

P – celoročný priemerný prepočítaný počet zamestnancov

T – celoročný priemerný prepočítaný počet riešiteľov projektov

O – celoročný priemerný prepočítaný počet obslužného personálu podieľajúceho sa na riešení projektov (technikov, laborantov, projektových manažérov a pod.) mimo zamestnancov v administratívnej, správnej a údržbovej budove, upratovačiek, vodičov a pod.

M, Ž – muži, ženy

Tabuľka 1b Štruktúra vedeckých pracovníkov (kmeňový stav k 31.12.2019)

Rodová skladba	Pracovníci s hodnotou				Vedeckí pracovníci v stupňoch		
	DrSc.	CSc./PhD.	prof.	doc.	I.	II.a.	II.b.
Muži	6	22	4	5	6	13	7
Ženy	2	13	0	1	2	6	7

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

Veková štruktúra (roky)	< 31		31-35		36-40		41-45		46-50		51-55		56-60		61-65		> 65	
	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
Muži	2	2.0	6	5.2	4	4.0	5	4.2	4	4.0	3	2.0	0	0.0	4	3.5	1	0.5
Ženy	1	1.0	0	0.0	1	0.6	5	5.0	2	2.0	3	3.0	0	0.0	3	3.2	0	0.0

A - Prepočet bez zohľadnenia úväzkov zamestnancov

B - Prepočet so zohľadnením úväzkov zamestnancov

Tabuľka 1d Priemerný vek zamestnancov organizácie k 31.12.2019

	Kmeňoví zamestnanci	Vedeckí pracovníci	Riešitelia projektov
Muži	45.9	44.7	44.8
Ženy	48.6	45.0	47.7
Spolu	47.3	44.8	45.8

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 2019 nezaznamenal žiadne zásadné zmeny v organizačnej štruktúre, avšak zaznamenali sme nezvyčajne rozsiahlu personálnu zmenu a obmenu. V priebehu roka dve pracovníčky odišli pracovať do priemyslu, traja pracovníci odišli ku koncu roka do dôchodku. Ďalšie personálne zmeny súviseli s odchodom pracovníkov zamestnaných na čiastočný úväzok. Všetkých päť pracovných pozícií na plný úväzok sa nám však podarilo nanovo obsadiť.

Prepočítaný počet pracovníkov v roku 2019 je na úrovni 57.38 FTE, čo je nižší stav v porovnaní s rokom 2018 (62,2). Do tohto počtu vstupujú aj zamestnanci platení z projektov APVV a jeden štipendista v programe IF MC. V roku 2019 bol priemerný vek všetkých pracovníkov ústavu 47,3 roka a priemerný vek vedeckých pracovníkov 44,8. Vzhľadom na to, že nedochádza k plynulej generačnej výmene, postupne sa zvyšuje aj priemerný vek zamestnancov. Napriek tomu, že zamestnávanie mladých schopných post-doktorandov na ústave je jednou z hlavných priorít, nevieme ju v požadovanej miere primerane 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. Tento fakt doteraz nebol pri tvorbe rozpočtu, hlavne mzdových fondov ústavov, zohľadnený. Preto vítame pripravovanú zmenu mzdovej politiky SAV.

Ústav sa od roku 2008 podieľal na realizácii 13-tich projektov financovaných zo ŠF EÚ, ktoré sú aktuálne všetky ukončené. Aj napriek tomu, administratívne zaťaženie na ich monitoring ostáva, pričom mzdové náklady na túto administráciu už nie je možné vykrývať z projektov, ale len zo mzdového fondu ústavu. Navyše, výraznú časť administratívnych výkonov preberajú aj vedeckí pracovníci.

Dňa 11.6.2019 ústav navštívili vybraní členovia predsedníctva s cieľom prerokovať akčný plán ústavu. Na stretnutí so zamestnancami ústavu odznali z obidvoch strán pozitívne aj kritické hodnotenia.

2. Vedecká činnosť

2.1. Domáce projekty

Tabuľka 2a Domáce projekty riešené v roku 2019

ŠTRUKTÚRA PROJEKTOV	Počet		Čerpané financie (€)					
	A	B	A				B	
			Zo zdrojov SAV		Z iných zdrojov		Zo zdrojov SAV	Z iných zdrojov
			Spolu	Pre ÚACH	Spolu	Pre ÚACH		
1. Projekty VEGA	10	2	95113	95113	-	-	7599	-
2. Projekty APVV	9	4	-	-	463686	332417	-	62560
3. Projekty OP ŠF	0	1	-	-	-	-	-	9867
4. Projekty SASPRO	0	0	-	-	-	-	-	-
5. Iné projekty (FM EHP, ŠPVV, Vedecko-technické projekty, ESF, na objednávku rezortov a pod.)	0	0	-	-	-	-	-	-

A - organizácia je nositeľom projektu

B - organizácia sa zmluvne podieľa na riešení projektu

Tabuľka 2b Domáce projekty podané v roku 2019

Štruktúra projektov	Miesto podania	Organizácia je nositeľom projektu	Organizácia sa zmluvne podieľa na riešení projektu
1. Účasť na nových výzvach APVV	-	7	2
2. Projekty výziev OP ŠF podané r. 2019	Bratislava Regióny		7

Projekty ŠF

Názov projektu: Rozvoj a podpora výskumno-vývojových aktivít Centra pre testovanie kvality a diagnostiku materiálov v oblastiach špecializácie RIS3 SK

Evidenčné číslo projektu: NFP313010W442

Acronym: CEDITEK II

Podávateľ projektu: Trenčianska univerzita Alexandra Dubčeka v Trenčíne

Partner/i: KONŠTRUKTA – Deference, a.s., MIKON spol. s r.o., Ústav anorganickej chémie SAV, Ústav materiálového výskumu SAV

Stav: podaný - odborné hodnotenie

Názov projektu: Gama radiačná záťaž sklovláknitých izolácií a bezpečné chladenie pri ťažkých haváriách v JE (GAĎAH)

Evidenčné číslo projektu: NFP313010V573

Acronym: GATAH

Podávateľ projektu: VÚEZ, a.s.

Partner/i: Fyzikálny ústav Slovenskej akadémie vied, Trenčianska univerzita Alexandra Dubčeka, Ústav anorganickej chémie SAV, Výskumný ústav chemických vlákien, a.s.,

Stav: podaný/doplnenie

Názov projektu: Výskum veľkokapacitného skladovania energie vo forme vodíka v geologických štruktúrach

Evidenčné číslo projektu: NFP313010V569

Acronym: EnStorH2

Podávateľ projektu: Ústav o Zemi Slovenskej akadémie vied

Partner/i: NAFTA a.s., Slovenská technická univerzita v Bratislave, Univerzita Komenského v Bratislave, Univerzita Pavla Jozefa Šafárika v Košiciach, Ústav anorganickej chémie SAV, Ústav geotechniky Slovenskej akadémie vied

Stav: podaný/administratívna kontrola

Názov projektu: Výskum využiteľnosti nekovových materiálov pre výrobu akumulátorov tepelenej energie a pre výrobu energetickej pilóty

Evidenčné číslo projektu: NFP313010V472

Acronym: (nie je uvedený v ITMS)

Podávateľ projektu: PREFA ALFA, a.s.

Partner/i: Slovenská technická univerzita v Bratislave, Technický a skúšobný ústav stavebný, n.o., Trenčianska univerzita Alexandra Dubčeka v Trenčíne, Ústav anorganickej chémie SAV, VUNAR a.s., ZTS INMART a.s.

Stav: podaný/administratívna kontrola

Názov projektu: Výskum efektívneho využitia plazmového pulzu pre konštrukciu nerotačného horizontálneho raziaceho systému v kryštalických horninách

Evidenčné číslo projektu: NFP313010V473

Podávateľ projektu: VUNAR a.s.

Partner/i: PREFA ALFA, a.s., Slovenská technická univerzita v Bratislave, Technický a skúšobný ústav stavebný, n.o., Ústav anorganickej chémie SAV, Ústav geotechniky Slovenskej akadémie vied, ZTS INMART a.s.

Stav: podaný/administratívna kontrola

Názov projektu: Výskum fyzikálnych, technických a materiálových aspektov rýchleho plynom chladeného reaktora IV. Generácie ALLEGRO

Evidenčné číslo projektu: NFP313010V444

Acronym: GAMA

Podávateľ projektu: VUJE, a.s.

Partner/i: Fyzikálny ústav SAV, Slovenská technická univerzita v Bratislave, Technická univerzita v Košiciach, Ústav anorganickej chémie SAV, Ústav materiálov a mechaniky strojov SAV, Ústav merania SAV, VÚEZ, a.s., YMS, a.s., Žilinská univerzita v Žiline

Stav: podaný/administratívna kontrola

Názov projektu: Materiály pre efektívnu výrobu, konverziu, transport, uskladnenie a bezpečné využívanie energie (M4E)

Evidenčné číslo projektu: NFP313010V453

Acronym: M4E

Podávateľ projektu: Univerzita Pavla Jozefa Šafárika v Košiciach

Partner/i: SPINEA Technologies s.r.o., Technická univerzita v Košiciach, Univerzita J. Seleyeho, Ústav anorganickej chémie SAV, Ústav experimentálnej fyziky SAV, Ústav geotechniky SAV, Ústav materiálového výskumu SAV, ZEOCEM, a.s.

Stav: podaný/administratívna kontrola

Projekty APVV – ÚACH SAV podávateľ

Názov projektu: Rozhranie fluoridová tavenina/tuhá (skelná) fáza: reakcie, štruktúra a charakterizácia (oxo)-(fluoro)-hlinitanov pre elektronické a fotonické aplikácie

Evidenčné číslo projektu: APVV-19-0301

Acronym: MISTRAL

Podávateľ projektu: ÚACH SAV

Partner/i: FÚ SAV

Stav: podaný

Názov projektu: Interakcia fluoridových taveninových systémov prvkov vzácnych zemín s oxidmi kritických prvkov v kontexte špeciálnych aplikácií.

Evidenčné číslo projektu: APVV-19-0270

Acronym: RARE

Podávateľ projektu: ÚACH SAV

Stav: podaný

Názov projektu: Kinetika korózie a štúdium morfológie natívneho povrchu úžitkového skla pomocou vyspelých spetkrálnych metód

Evidenčné číslo projektu: APVV-19-0014

Acronym: KIKOMO

Podávateľ projektu: ÚACH SAV (M. Chromčíková)

Partner/i: TnU AD (M. Liška)

Stav: podaný

Názov projektu: Bionanokompozitné materiály na báze organických polykatiónov a vrstevnatých silikátov

Evidenčné číslo projektu: APVV-19-0487

Acronym: BioPolSil

Podávateľ projektu: ÚACH SAV

Partner/i: ÚPo SAV

Stav: podaný

Názov projektu: Vývoj nnástrojov pre pokročilú analýzu a predikciu parametrov spektier EPR, NMR a pNMR komplexných systémov obsahujúcich ťažké prvky

Evidenčné číslo projektu: APVV-19-0516

Acronym: DKS-pNMR

Podávateľ projektu: UACH SAV (OlgaMalkin)

Partner/i: -

Stav: podaný

Projekty APVV – ÚACH SAV partner

Názov projektu: Anódy pre Li-iónové batérie na báze uhlík-kremíkových kompozitov

Evidenčné číslo projektu: APVV-19-0491

Acronym: ALICES

Podávateľ projektu: Centrum pre využitie pokročilých materiálov SAV

Partner/i: UACH SAV, FU SAV, UPo SAV, UMMS SAV,

Stav: podaný

Názov projektu: Bentonit: strategická surovina Slovenska - inovatívne hodnotenie zdrojov a ich kvality pre jej efektívne využívanie

Evidenčné číslo projektu: APVV-19-0260

Acronym: BEN3V

Podávateľ projektu: PríF UK

Partner/i: Ústav anorganickej chémie, Ústav vied o Zemi

Stav: podaný

Projekty APVV – bilaterálne

Názov projektu: Rozhranie fluoridová tavenina/tuhá fáza: reakcie a štruktúra (oxo)-(fluoro)- hlinitanov pre

elektronické aplikácie

Evidenčné číslo projektu: DS-FR-19-0037 (multilaterálna výzva APVV)**Acronym:** MOLIERE**Podávateľ projektu:** ÚACH SAV**Partner/i:** Conditions Extrêmes et Matériaux: Haute Temperature et Irradiation, CNRS, France, Ústav jaderné fyziky AV ČR, v. v. i., Řež, Česká Republika**Stav:** podaný**Názov projektu:** Percepcia spinovej interakcie na pokročilej úrovni**Evidenčné číslo projektu:** SK-FR-19-0001**Acronym:** SCALP**Podávateľ projektu:** ÚACH SAV (Olga Malkin)**Partner/i:** -**Stav:** schválený

2.2. Medzinárodné projekty

2.2.1. Medzinárodné projekty riešené v roku 2019

Tabuľka 2c Medzinárodné projekty riešené v roku 2019

ŠTRUKTÚRA PROJEKTOV	Počet		Čerpané financie (€)					
			A			B		
	A	B	Zo zdrojov SAV Spolu	Pre ÚACH	Z iných zdrojov Spolu	Pre ÚACH	Zo zdrojov SAV	Z iných zdrojov
1. Projekty 7. RP EÚ a Horizont 2020	1	0	-	-	60717	60717	-	-
2. Projekty ERA.NET, ESA, JRP	0	1	-	-	-	-	-	11502
3. Projekty COST	0	0	-	-	-	-	-	-
4. Projekty EUREKA, NATO, UNESCO, CERN, IAEA, IVF, ERDF a iné	0	0	-	-	-	-	-	-
5. Projekty v rámci medzivládnych dohôd	0	0	-	-	-	-	-	-
6. Bilaterálne projekty MAD	1	0	-	-	-	-	-	-
7. Bilaterálne projekty ostatné	4	1	48996	48996	-	-	-	-
8. Podpora MVTS z národných zdrojov okrem SAV (APVV a iné)	2	0	-	-	6153	6153	-	-
9. Iné projekty	0	0	-	-	-	-	-	-

A - organizácia je nositeľom projektu

B - organizácia sa zmluvne podieľa na riešení projektu

2.2.2. Medzinárodné projekty Horizont 2020 podané v roku 2019

Tabuľka 2d Počet projektov Horizont 2020 v roku 2019

	A	B
Počet podaných projektov Horizont 2020	1	1

A - organizácia je nositeľom projektu

B - organizácia sa zmluvne podieľa na riešení projektu

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

Názov projektu: New generation of eco-friendly ionic liquids for high efficient electrochemical treatment of metals and alloys**Evidenčné číslo projektu, výzva:** 886867 (MSCA-IF-2019/MSCA-IF-EF-2019)

Acronym: NGETMA**Uchádzač:** Anna Kityk**Koordinátor ÚACH:** M. Boča**Stav:** podaný**Názov projektu:** Eco-friendly composites - mine tailings based geopolymers**Program:** ERA.MIN2 Acronym: ECOMINING**Podávateľ projektu:** Cracow University of Technology, Poľsko**Koordinátor ÚACH:** P. Tatarko

Ďalší partneri: University of Aveiro (Portugalsko), Universitatea Babeş-Bolyai Cluj-Napoca (Rumunsko), Nigde Ömer Halisdemir University Nigde (Turecko), La Pontificia Universidad Católica de Chile, Santiago (Čile), Ekologia Przedsiębiorczość Inowacje, Czestochowa (Poľsko), Przedsiębiorstwo BudowlanoProdukcyjne, Krakow, (Poľsko), Geomaterials Valorization Innovation P.C., (Grécko), University of Patras (Grécko), Santa Catarina Extreme South University (Brazília), Slovenian National Building and Civil Engineering Institute, Ljubljana (Slovinsko)

Stav: zamietnutý

2.2.3. Zámery na čerpanie štrukturálnych fondov EÚ v ďalších výzvach

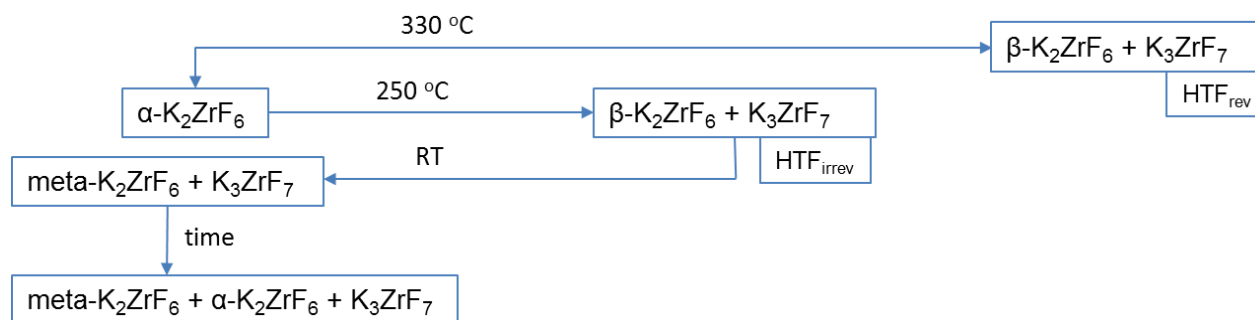
2.3. Najvýznamnejšie výsledky vedeckej práce (maximálne 1000 znakov + 1 obrázok; bibliografický údaj uvádzajte rovnako ako v zozname publikačnej činnosti, vrátane IF)

2.3.1. Základný výskum

Nezvyčajná modifikačná premena zlúčeniny K_2ZrF_6 .

Riešitelia z ÚACH SAV: BOČA, Miroslav – NETRIOVÁ, Zuzana – KUBÍKOVÁ, Blanka – HRUŠKA, Branislav – LIŠKA, Marek – CHROMČÍKOVÁ, Mária – VASKOVÁ, Zuzana

Zlúčenina α - K_2ZrF_6 podlieha nezvyčajnej viacstupňovej modifikačnej premene v tuhom stave. Táto modifikačná premena môže byť reverzibilná alebo ireverzibilná vzhľadom na cieľovú teplotu. Zahrievanie K_2ZrF_6 na 250 °C spôsobuje nevratnú modifikačnú premenu. Starnutie takejto zmesi podlieha ďalšiemu procesu premien. Proces transformačných premien bol sledovaný rôznymi metódami ako DTA, DSC, ^{19}F MAS NMR, XRD, tepelnou difúziou ako aj Ramanovou spektroskopiou pri rôznych teplotných režimoch pričom získané spektrá boli následne analyzované pomocou Principal Component Analysis (PCA) a Multivariate Curve Resolution (MCR) metód. Štatistická analýza Ramanových spektier potvrdila ireverzibilný charakter α – HTF_{irrev} transformácie. Navyše transformácia HTF_{rev} fázy na α fázu si vyžaduje prítomnosť aj HTF_{irrev} fázy. Zaujímavosťou je aj to, že odozva monitorovania modifikačných premien rôznymi technikami vykazovala neočakávané odozvy, ktoré bolo treba interpretovať. Obrázok sumarizuje schému transformačných premien navrhnutých na základe získaných experimentálnych výsledkov.



Publikácie

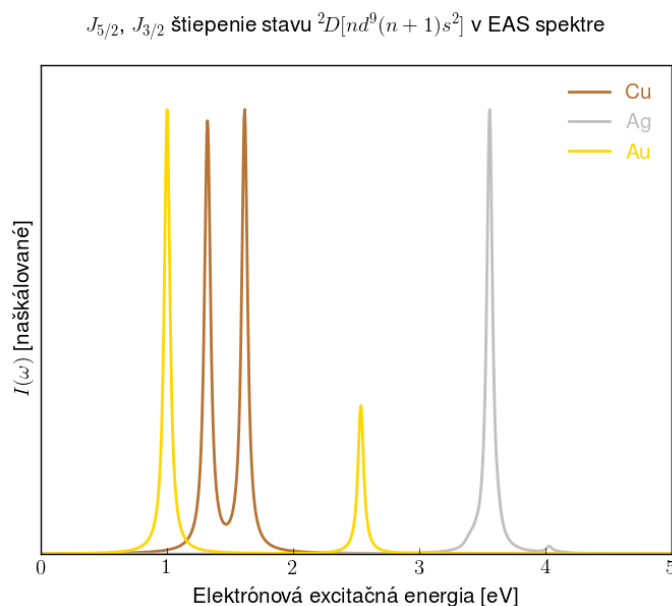
BOČA, Miroslav** – NETRIOVÁ, Zuzana – RAKHMATULLIN, Aydar – VASKOVÁ, Zuzana – HADZIMOVÁ, Eva – SMRČOK,

Ľubomír – HANZEL, Ondrej – KUBÍKOVÁ, Blanka. The differing responses of various techniques in measuring the phase transformations of K₂ZrF₆. In Journal of Molecular Liquids, 2019, vol. 287, p. 110969-1-110969-10. (4.561 – IF2018).
HRUŠKA, Branislav** – NETRIOVÁ, Zuzana – VASKOVÁ, Zuzana – BOČA, Miroslav – CHROMČÍKOVÁ, Mária – LIŠKA, Marek. High-temperature Raman study of K₂ZrF₆ phase transitions. In Journal of Alloys and Compounds, 2019, vol. 791, p. 45-50. (4.175 – IF2018).

Presné modelovanie elektrónových absorpčných spektier systémov s uzavretým aj otvoreným obalom.

Riešiteľ z ÚACH SAV: KOMOROVSKÝ, Stanislav

Presná predpoveď elektrónových absorpčných spektier zlúčenín obsahujúcich ťažké prvky vyžaduje správne zohľadnenie relativistických efektov. Vhodné započítanie týchto efektov je napríklad nevyhnutné pri opise fotochemických vlastností organických diód emitujúcich svetlo, pri predikcii röntgenových L-edge spektier, alebo iných javoch súvisiacich so spinovými efektami v magnetických materiáloch. V tejto práci sme vyvinuli štvorzložkovú (4c) metódu výpočtu excitačných energií v rámci časovo závislej teórie funkcionálu hustoty (TDDFT). Metóda 4c-TDDFT je použiteľná na systémoch obsahujúcich atómy s ľubovoľným atómovým číslom a jej efektívna implementácia v našom programe ReSpect umožňuje rutinné výpočty na reálnych systémoch s až 200 atómami. Okrem toho sa metóda 4c-TDDFT dá použiť na referenčné stavy s uzavretým aj otvoreným obalom. V prípade 4c metód pre systémy s otvoreným obalom je to vôbec prvá úspešná implementácia vo svete. Tento úspech je pozoruhodný hlavne preto, že vedecká obec doteraz túto úlohu považovala za príliš náročnú. Napríklad autori článku [Mol. Phys. 111, 3741 (2013)] napísali: „... ktorého [4c-TDDFT] momentálna adaptácia je technicky príliš náročná, ak nie nemožná. ...”. Učebnicová demonštrácia metódy na systémoch s otvoreným obalom je výpočet spin-orbitálneho štiepenia $J_{5/2}$, $J_{3/2}$ inak desaťkrát degenerovaného 2D stavu.



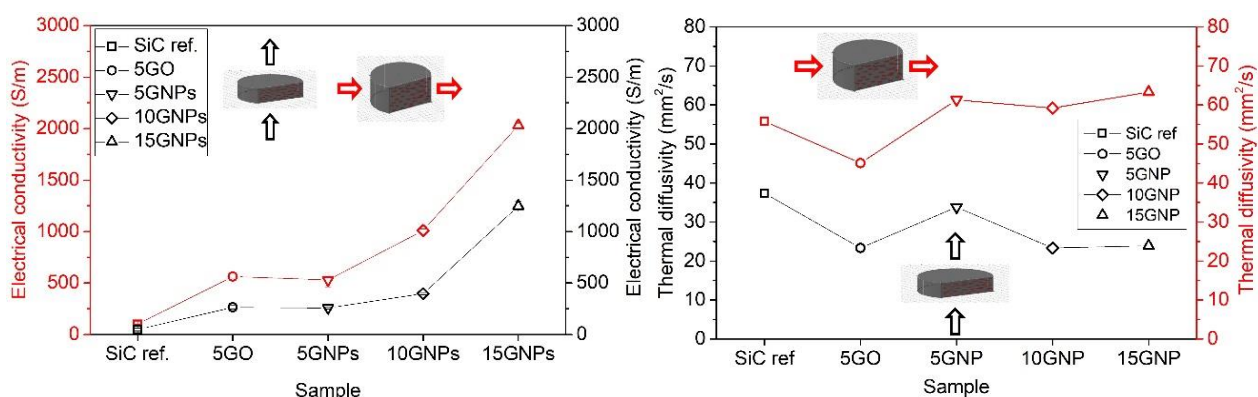
Publikácie

KOMOROVSKÝ, Stanislav – CHERRY, Peter – REPISKÝ, Michal. Four-component relativistic time-dependent density-functional theory using a stable noncollinear DFT ansatz applicable to both closed- and open-shell systems. In Journal of Chemical Physics, 2019, vol. 151, no. 18, p. 184111-1-184111-14. (2.997 – IF2018).

Elektro-iskrovo obrábatel'né SiC s grafénovými nanoplatničkami (GNPs) a oxidom grafénu (GO) ako elektricky vodivými fázami

Riešitelia z ÚACH SAV: HANZEL, Ondrej – ŠAJGALÍK, Pavol

Hutné kompozitné materiály na báze SiC s prídavkami Y_2O_3 a Al_2O_3 ako spekacími prísadami a s prídavkom 5 – 15 hm. % grafénových nanoplatničiek (GNPs) alebo 5 hm. % oxidu grafénu (GO) boli pripravené metódou Rapid hot press pri teplote 1800°C , pri tlaku 50 MPa po dobu 5 minút vo vákuu. Anizotropia mikroštruktúry ako dôsledok usporiadania grafénových vrstiev v smere kolmom na lisovací tlak bola potvrdená meraním elektrickej vodivosti a tepelnej difuzivity. Najvyššia hodnota elektrickej vodivosti (2031 S/m) bola dosiahnutá pri kompozite s 15 hm. % grafénových platničiek v smere rovnobežnom na grafénové roviny, zatiaľ čo v smere kolmom na orientáciu grafénových vrstiev bola elektrická vodivosť iba 1246 S/m . Rýchlosť odoberania materiálu pri elektro-iskrovom obrábaní bola pri všetkých SiC-GNP a SiC-GO kompozitoch vyššia ako $1.6 \text{ mm}^3/\text{min}$. Takmer dvojnásobná rýchlosť odoberania materiálu ($2.8 \text{ mm}^3/\text{min}$) bola dosiahnutá pre kompozity obsahujúce 15 hm. %, pričom zároveň drsnosť povrchov po obrábaní klesla na $1.5 \mu\text{m}$.



Elektrická vodivosť a tepelná difúzivita kompozitných materiálov SiC-GNP a SiC-GO meraná v smere kolmom a rovnobežnom na uloženie grafénových vrstiev.

Publikácie:

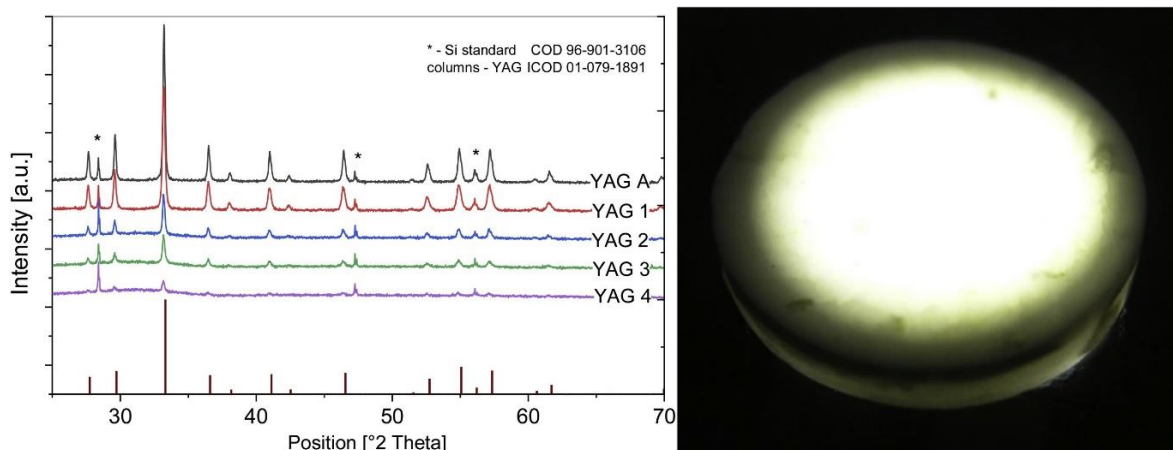
HANZEL, Ondrej - SINGH, Meinam Annebushan - MARLA, Deepak - SEDLÁK, Richard - ŠAJGALÍK, Pavol. Wire electrical discharge machinable SiC with GNPs and GO as the electrically conducting filler. In Journal of the European Ceramic Society, 2019, vol. 39, no. 8, p. 2626-2633. (4.029 - IF2018).

2.3.2. Aplikačný typ

Príprava translucetnej YAG sklo/keramiky pri teplotách pod 900°C

Riešitelia z ÚACH SAV: MICHÁLKOVÁ, Monika – GALUSEK, Dušan

Hutná translucetná sklokeramika so zložením yttrito-hlinitého granátu (YAG) sa pripravila zo sklenených mikrogulôčok so zložením YAG. Mikrogulôčky sa zhutnili do kusového materiálu v žiarovom lise spekaním viskóznym tokom. Vďaka kontrolovanej kryštalizácii bolo možné pripraviť YAG sklo-keramiku s rôznym obsahom amorfnej fázy. Po zhutnení dosahovala čistá YAG keramika relatívnu hustotu nad 94 % pri teplote iba 891°C , zatiaľ čo sklo-keramika dosiahla relatívnu hustotu nad 99 % pri teplote 815°C bez izotermickej výdrže. Dopovaná YAG keramika sa v súčasnosti využíva v laseroch napr. v lekárstve (konkrétne v chirurgii ako presný a šetrný spôsob rezania a odparovania tkaniva, napríklad pri operáciách očnej sietnice) alebo v oblasti spracovania kovových i nekovových materiálov.

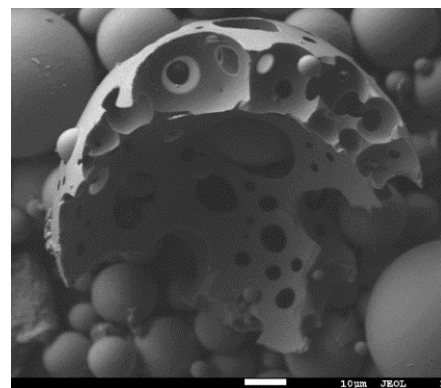
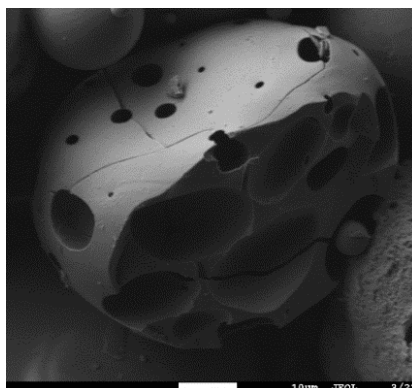
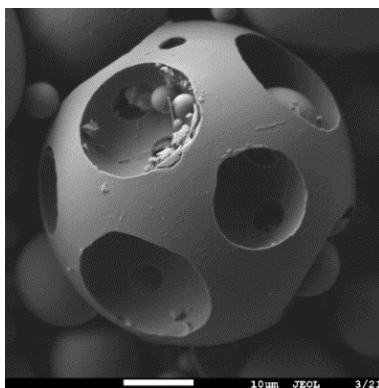
**Publikácie:**

MICHÁLKOVÁ, Monika - KRAXNER, J. – MICHÁLEK, M. – GALUSEK, Dušan Preparation of translucent YAG glass/ceramic at temperatures below 900 °C. Journal of the European Ceramic Society, IF: 4,029, In Press, Corrected Proof Available online 5 November 2019 <https://doi.org/10.1016/j.jeurceramsoc.2019.11.011>

2.3.3. Medzinárodné vedecké projekty**Pórovité bioaktívne sklenené mikrogulôčky pripravené plameňovou syntézou**

Riešiteľ z ÚACH SAV: GALUSEK, Dušan

Vyvinula sa technológia nízko-nákladovej prípravy pórovitých bio-aktívnych sklenených mikrogulôčok. Sklený prášok so zložením bioskla 45S5 s nepravidelným tvarom častíc sa pripravil konvenčným tavením a následne sa povrch častíc alkalicky aktivoval. Alkalická aktivácia zabezpečila tvorbu pórov ako na povrchu mikrogulôčiek, tak aj v ich vnútri (Obrázok). Výsledné mikrogulôčky majú priemer medzi 45 a 75 μm , a nájdu uplatnenie pri regenerácii kostí v tkanivovom inžinierstve. Vďaka svojej pórovitosti môžu slúžiť aj na prepravu liečiv v ľudskom tele.

**Publikácie:**

KRAXNER, Jozef - MICHÁLEK, Martin - ROMERO, Acacio R. - ELSAYED, H. - BERNARDO, E. - BOCCACCINI, Aldo - GALUSEK, Dušan. Porous bioactive glass microspheres prepared by flame synthesis process. In Materials Letters, 2019, vol. 256, p. 126625-1-126625-4. (2018: 3.019 - IF, Q2 - JCR).

Optimalizácia syntézy nanokryštalického Fe_2O_3 na povrchu kompozitných pórovitých anorganických materiálov na báze ílových minerálov: využitie v katalytickej reakcii pre rozklad toluénu.

Riešitelia z ÚACH SAV:

Pórovité anorganické materiály na báze ílových minerálov, tzv. PCH predstavujú zaujímavú alternatívu k rôznym štruktúram na báze SiO_2 . Cieľom práce bolo navrhnuť syntézu a optimalizovať jej podmienky a

pripraviť kompozitný materiál PCH/FeO_x s vysokou efektivitou v reakcii rozkladu toluénu. Odbúravaniu prchavých organických látok (VOC) a ich rozkladu na zlúčeniny z menším negatívnym dopadom na životné prostredie sa venuje veľká pozornosť a použitie Fe-PCH sa študovala ako lacnejšia alternatíva ku katalyzátorom na báze oxidov ušľachtilých kovov. Pripravené Fe-PCH obsahovali nanoštruktúrne formy α -Fe₂O₃ and Fe₃O₄ oxidov s rôznou distribúciou častíc, ale aj pomerom Fe-fáz v závislosti na podmienkach syntézy (koncentrácia FeCl₃, ktorý sa použil ako zdroj Fe³⁺, tlak, čas impregnácie a kalcinácie). Železo v oktaedrickej koordinácii α -Fe₂O₃ bolo efektívne pre zvýšenie aktivity katalyzátora, zatiaľ čo Fe₃O₄ nanokryštály aktivitu znižovali. Práca poskytla originálne interpretácie zmien IČ spektrách v ďalekej oblasti s podporou DFT výpočtov, čím sa potvrdila prítomnosť α -Fe₂O₃ a Fe₃O₄ fáz na povrchu Fe-PCH.

Publikácie:

ZIMOWSKA, M. - GURGUL, J. - SCHOLTZOVA, E. - SOCHA, R.P. - PÁLKOVÁ, H. - LITYNSKA-DOBRYNSKA, L. - MORKZYCKI, L. - LATKA, K. A precursor approach for the development of lace-like Fe₂O₃ nanocrystallites triggered by pressure dependent nucleation and growth of akaganeite over clay based composites for toluene combustion. In Journal of Physical Chemistry C, 2019, vol. 123, no. 43, p. 26236-26250. (4.309 - IF2018).

Spoločný projekt v rámci medziakademickej dohody medzi Poľskou akadémiou vied a SAV (Polish-Slovak joint research project under the PAS-SAS agreement 2016-2018)

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

Tabuľka 2e Štatistika vybraných kategórií publikácií

PUBLIKAČNÁ A EDIČNÁ ČINNOSŤ	Počet v r. 2019/ doplňky z r. 2018
1. Vedecké monografie a monografické štúdie vydané v domácich vydavateľstvách (AAB, ABB)	0 / 0
2. Vedecké monografie a monografické štúdie vydané v zahraničných vydavateľstvách (AAA, ABA)	0 / 0
3. Odborné monografie, vysokoškolské učebnice a učebné texty vydané v domácich vydavateľstvách (BAB, ACB, CAB)	0 / 0
4. Odborné monografie a vysokoškolské učebnice a učebné texty vydané v zahraničných vydavateľstvách (BAA, ACA, CAA)	0 / 0
5. Kapitoly vo vedeckých monografiách vydaných v domácich vydavateľstvách (ABD)	0 / 0
6. Kapitoly vo vedeckých monografiách vydaných v zahraničných vydavateľstvách (ABC)	0 / 0
7. Kapitoly v odborných monografiách, vysokoškolských učebniciach a učebných textoch vydaných v domácich vydavateľstvách (BBB, ACD)	0 / 0
8. Kapitoly v odborných monografiách, vysokoškolských učebniciach a učebných textoch vydaných v zahraničných vydavateľstvách (BBA, ACC)	0 / 0
9. Vedecké práce registrované v Current Contents Connect (ADCA, ADCB, ADDA, ADDB)	44 / 0
10. Vedecké práce registrované vo Web of Science Core Collection alebo Scopus (ADMA, ADMB, ADNA, ADNB)	5 / 0
11. Vedecké práce v ostatných domácich časopisoch (ADFA, ADFB)	0 / 0
12. Vedecké práce v ostatných zahraničných časopisoch (ADEA, ADEB)	0 / 0
13. Vedecké práce v domácich recenzovaných zborníkoch (AEDA)	0 / 0
14. Vedecké práce v zahraničných recenzovaných zborníkoch (AECA)	0 / 0
15. Publikované príspevky na domácich vedeckých konferenciách (AFB, AFD)	19 / 0
16. Publikované príspevky na zahraničných vedeckých konferenciách (AFA, AFC)	7 / 0
17. Vydané periodiká evidované v CCC, WoS Core Collection, SCOPUS	0
18. Ostatné vydané periodiká	0
19. Zostavovateľské práce knižného charakteru (FAI)	2 / 0
20. Preklady vedeckých a odborných textov (EAJ)	0 / 0
21. Heslá v odborných terminologických slovníkoch a encyklopédiách (BDA, BDB)	0 / 0
22. Recenzie v časopisoch a zborníkoch (EDI)	0 / 0

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

Tabuľka 2f Štatistika vedeckých prác podľa kvartilu vedeckého časopisu

Kvartil vedeckého časopisu	Q1	Q2	Q3	Q4	Spolu
Podľa IF z r. 2018 (zdroj JCR) <i>Počet článkov / doplnky 2017</i>	31 / 0	8 / 0	7 / 0	0 / 0	46 / 0
Podľa SJR z r. 2018 (zdroj Scimago) <i>Počet článkov / doplnky 2017</i>	35 / 0	7 / 0	3 / 0	4 / 0	49 / 0

Tabuľka 2g Ohlasy

OHLASY	Počet v r. 2018/ doplnky z r. 2017
Citácie vo WOS (1.1, 2.1)	1528 / 23
Citácie v SCOPUS (1.2, 2.2)	24 / 5
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)	2 / 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	53
Prednášky a vývesky na domácich vedeckých podujatiach	38

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. – ŠIMURDA M. – ŠVEC P. – ŠVEC P. Jr. – JANIČKOVIČ D. – CZÍMEROVÁ A. – KUBÍKOVÁ B. – MLYNÁRIKOVÁ J. Unusual phase transformations in ternary fluoride systems. In 19th European Symposium on Fluorine Chemistry, Warszawa, Poľsko, dátum konferencie Oficyna Wydawniczo-Poligraficzna ADAM, 2019, p. 134.

BUJDÁK J. The phenomena occurring in the systems of layered silicates and organic dyes. Research Work and Collaboration Symposium: Molecules and Materials for Life, Téma: Interaction of Inorganic Clusters, Cages, and Containers with Light, Villa Lanna v Prahe, Česká republika, 19.3. 2019

BUJDÁK J. Energy transfer between dye molecules in the hybrid materials with layered silicates. Research Work and Collaboration Symposium: Molecules and Materials for Life, Téma: Interaction of Inorganic Clusters, Cages, and Containers with Light, Liblice, Česká republika, 5.12. 2019.

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

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

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

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

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

PRNOVÁ A. – VALÚCHOVÁ J. – DOHNALOVÁ Ž. – HANZEL O. – KLEMENT R. – BRUNEEL E. – GALUSEK D. Preparation of Al₂O₃-Y₂O₃ glass microspheres; influence of particle size distribution on thermal behavior of prepared systems., Konferencie o špeciálnych anorganických pigmentoch a práškových materiáloch, 18. september 2019, Pardubice, ČR

SCHOLTZOVÁ E. - JANKOVIČ Ľ. - ŠKORŇA P. - MORENO RODRÍGUEZ D. - TUNEGA D. Insight into

the stability of beidellite intercalates. In BIT's 7th Annual Conference of AnalytiX-2019, 12 – 14- apríl 2019, Singapore, Exploring Innovative Advances and Applications, p. 78.

ŠAJGALÍK P. Porous silicon nitride: A material for the bioactive composite implants. In ICACC 2019. 43rd International Conference & Exposition on Advanced Ceramics and Composites, January 27 - February 1, 2019, Daytona Beach, Florida, USA, 27. 1- 1.2.2019

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

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

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

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

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

2.6.2. Vyžiadané prednášky na domácich vedeckých podujatiach

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

MALKIN, V. - MALKINA, O. Calculations and interpretation of the EPR parameters in the framework of 2- and 4-component DFT approach. In XIth EFEP 2019 Conference: book of abstracts. - Bratislava: Vydavateľstvo SCHK, 2019, pL6, 1 p. ISBN 978-80-8208-020-2.

2.6.3. Vyžiadané prednášky na významných vedeckých inštitúciách

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

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

BUJDAK J. Photophysical phenomena occurring in hybrids of expandable phyllosilicates and organic dyes. Bayreuth, Univerzita v Bayreuth, Nemecko, 25. január 2019

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

CHROMČÍKOVÁ M. – HRUŠKA B. – LIŠKA M. Získanie hodnotných dát analýzou nevydarených termodynamických experimentov. Termoanalytický seminár, Brno, Česká republika, 10. november 2019

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

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

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

MALKIN O. – KOMOROVSKÝ S. – MALKIN V. Beyond the Dirac vector model?, Technická Univerzita v Berlíne, Nemecko, 3. december 2019

PRNOVÁ A. – VALÚCHOVÁ J. – PARCHOVIANSKY M. – KLEMENT R. – GALUSEK D. HP sintering of yttrium aluminate glasses, impact of particle size on mechanical properties, Univerzita v Gente, Belgicko, november 2019

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

TATARKO P. Field assisted processing for the development and joining of ceramics for extreme environments, Ningbo Institute of Materials Technology and Engineering (NIMTE), Chinese Academy of Sciences, Ningbo, Čína, 8. november 2019

2.7. Patentová a licenčná činnosť na Slovensku a v zahraničí v roku 2019

2.7.1. Vynálezy, na ktoré bol v roku 2019 udelený patent

- a) na Slovensku
- b) v zahraničí

2.7.2. Vynálezy prihlásené v roku 2019

- 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 2019
- b) udelené v roku 2019

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 2019 a súčet za predošlé roky sa neuvádzajú, 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
Hnatko Miroslav	VEGA	1
Komorovský Stanislav	VEGA	1
Korenko Michal	APVV VV 2019	2
	DoktorGrant	8
Pavlík Viliam	OPVaI-VA/DP/2018/1.1.2-01	3
	OPVaI-VA/DP/2018/1.1.3-04	1
	OPVaI-VA/DP/2018/1.1.3-07	1
Tatarko Peter	MVTS: SAS-NASU	1

2.9. Účasť na spracovaní hesiel do encyklopédie Beliana

Počet autorov hesiel: 0

2.10. Recenzovanie publikácií a príspevkov vo vedeckých časopisoch

Tabuľka 2j Počet recenzovaných monografií, článkov, zborníkov

Meno pracovníka	Knižné 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
Boháč Peter	0	0	2	0	0	0	0
Bujdák Juraj	0	0	5	0	0	0	10
Galusek Dušan	0	0	6	0	0	0	0
Hanzel Ondrej	0	0	1	0	0	0	0
Hnatko Miroslav	0	0	0	0	0	8	0
Komorovský Stanislav	0	0	1	0	0	0	0
Kubíková Blanka	0	0	1	0	0	0	0
Lenčees Zoltán	0	0	31	0	0	0	0
Madejová Jana	0	0	6	0	0	0	0
Malkin Oľga	0	0	2	0	0	0	0
Páľková Helena	0	0	2	0	0	0	0
Pavlík Viliam	0	0	5	0	0	0	0
Sedláček Jaroslav	0	0	3	0	0	0	0
Scholtzová Eva	0	0	6	0	0	0	0
Tatarko Peter	0	0	23	0	0	4	0
Tatarková Monika	0	0	2	0	0	0	0
Spolu	0	0	98	0	0	12	10

2.11. Iné informácie k vedeckej činnosti.

Počet časopiseckých karentovaných publikácií registrovaných v databáze WOS a SCOPUS v roku 2019 dosiahol číslo 44. 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 39,71, vrátane deviatich doktorandov (piatich s plnou kapacitou, štyria s kapacitou 0,3 pri zohľadnení dátumu ich nástupu na štúdium 1.9.2019), ktorí k 31.12. vystupovali v riešiteľských kolektívoch 45,91. Potom na jedného pracovníka pripadá 1,11 karentovanej publikácie, vrátane doktorandov – 0,96 publikácie.

Takýto stav nepovažujeme za dostatočný a cieľom naďalej ostáva dosiahnuť dve publikácie na vedeckého pracovníka ročne, ktorý zodpovedá štandardu vyspelých vedeckých pracovísk s podobným zameraním. Priemerný impakt faktor časopisov, v ktorých boli práce uverejnené, bol 3,69, pokiaľ vlani to bolo 3,41 (treba mať na pamäti, že údaje sú zo záverečných správ, v ktorých sa nachádzajú aj doplnky publikácií za predchádzajúci rok 2018, ktorým ešte neboli priradené kompletne bibliografické údaje v čase spracovávaní podkladov do záverečných správ).

Citovanosť (vo všetkých dostupných databázach WOS – 1551, SCOPUS – 29) na vedeckého pracovníka (34,93) je 45,23 citácií, čo predstavuje nárast v porovnaní s rokom 2018. Pracovníci ústavu predniesli 16 pozvaných prednášok na významných svetových konferenciách.

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

3.1. Údaje o doktorandskom štúdiu

Tabuľka 3a Počet doktorandov v roku 2019

Forma	Počet k 31.12.2019				Počet doktorandov po doktorandskej skúške		Počet ukončených doktorantúr v r. 2019					
							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	6	3	2	2	4	1	1	0	1	1	0	0
Denná z iných zdrojov	0	0	0	0	0	0	0	0	0	0	0	0
Externá	0	0	0	0	0	0	0	0	0	0	0	0
Spolu	6	3	2	2	4	1	1	0	1	1	0	0
Súhrn	9		4		5		1		2		0	

Uvádzajte len doktorandov organizácie ako externej vzdelávacej inštitúcie.

Riadok „Spolu“ je súčtom troch riadkov nad ním. Každá bunka v „Súhrn“ je súčtom dvoch buniek nad ňou. V stĺpci „Počet doktorandov po doktorandskej skúške“ sa uvádza počet doktorandov, ktorí počas roku 2019 boli aspoň 1 deň doktorandami po doktorandskej skúške. Sú číselne zahrnutí aj v predchádzajúcich stĺpcoch.

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 2019 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
-----------------	----------	---------------------------	----------------------	---------------------------------	------------------------------	-----------------------------------

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

Tabuľka 3d Menný zoznam ukončených doktorandov v roku 2019 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 hodnotu
Ing. Michal Slaný	interné štúdium hradené z prostriedkov SAV	9 / 2014	8 / 2019	5.2.19 anorganická technológia a materiály	RNDr. Jana Madejová DrSc., Ústav anorganickej chémie SAV	Fakulta chemickej a potravinárskej technológie STU

3.5. Uplatnenie absolventov doktorandského štúdia

Tabuľka 3e Prehľad uplatnenia absolventov doktorandského štúdia

Počet absolventov PhD. štúdia v roku 2019 (obhajoba leto 2019)	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
1	1	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	DEU/1, ESP/1, GRC/1, IND/1, TUR/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	Doktorandské štúdium uskutočňované na (univerzita/vysoká škola a fakulta)
chemická fyzika	4.1.11	Univerzita Komenského v Bratislave
anorganická chémia	4.1.15	Prírodovedecká fakulta UK
anorganická technológia a materiály	5.2.19	Slovenská technická univerzita v Bratislave

Tabuľka 3h Účasť na pedagogickom procese

Menný prehľad pracovníkov, ktorí boli menovaní do spoločných odborových komisií pre doktorandské štúdium	Menný prehľad pracovníkov, ktorí pôsobili ako členovia vedeckých rád univerzít, správnych rád univerzít a fakúlt	Menný prehľad pracovníkov, ktorí získali vyššiu vedeckú, pedagogickú hodnosť alebo vyšší kvalifikačný stupeň
doc. Ing. Miroslav Boča, DrSc. (anorganická chémia)	doc. Ing. Miroslav Boča, DrSc. (Fakulta chemickej a potravinárskej technológie STU)	Mgr. Tímea Baranyaiová, PhD. (PhD., Prírodovedecká fakulta UK)
doc. Ing. Miroslav Boča, DrSc. (anorganická technológia a materiály)	doc. Ing. Miroslav Boča, DrSc. (Trenčianska univerzita Alexandra Dubčeka v Trenčíne)	doc. Ing. Mária Chromčíková, PhD. (doc., Trenčianska univerzita Alexandra Dubčeka v Trenčíne)
doc. Ing. Miroslav Boča, DrSc. (odbor v zahraničí)	prof. Ing. Dušan Galusek, DrSc. (Fakulta špeciálnej techniky TnUAD)	Mgr. Marek Pribus, PhD. (PhD., Prírodovedecká fakulta UK)
prof. RNDr. Juraj Bujdák, DrSc. (anorganická chémia)	prof. Ing. Dušan Galusek, DrSc. (Fakulta zdravotníctva TnUAD)	Ing. Michal Slaný, PhD. (PhD., Fakulta chemickej a potravinárskej technológie STU)
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. (Fakulta chemické technológie VŠCHT, Praha, ČR)	

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

3.8. Údaje o pedagogickej činnosti

Tabuľka 3i Prednášky a cvičenia vedené v roku 2019

PEDAGOGICKÁ ČINNOSŤ	Prednášky		Cvičenia a semináre	
	doma	v zahraničí	doma	v zahraničí
Počet prednášateľov alebo vedúcich cvičení	4	3	5	0
Celkový počet hodín v r. 2019	57	34	140	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	3
2.	Počet vedených alebo konzultovaných diplomových a bakalárskych prác	3
3.	Počet pracovníkov, ktorí pôsobili ako školitelia doktorandov (PhD.)	11
4.	Počet školených doktorandov (aj pre iné inštitúcie)	19
5.	Počet oponovaných dizertačných a habilitačných prác	12
6.	Počet pracovníkov, ktorí oponovali dizertačné a habilitačné práce	4
7.	Počet pracovníkov, ktorí pôsobili ako členovia komisií pre obhajoby DrSc. prác	1
8.	Počet pracovníkov, ktorí pôsobili ako členovia komisií pre obhajoby PhD. prác	7
9.	Počet pracovníkov, ktorí pôsobili ako členovia komisií, resp. oponenti v inauguračnom alebo habilitačnom konaní na vysokých školách	2

3.9. Iné dôležité informácie k pedagogickej činnosti

ÚACH SAV aj v roku 2019 vyvinul enormnú iniciatívu k získaniu nových doktorandov. V spolupráci s dvoma vysokými školami (PriF UK a FChPT STU) celkovo vypísal 19 tém v troch študijných programoch (4.1.15 Anorganická chémia, 5.2.19 Anorganické technológie a materiály a 4.1.11 Chemická fyzika.), ktoré okrem príslušných akademických informačných systémov, boli zverejnené aj na medzinárodných portáloch. Dva z týchto portálov boli samostatnou iniciatívou ÚACH SAV. Na základe úspešného prijímacieho konania Ústav anorganickej chémie prijal zo 6 kandidátov, 5 študentov, z ktorých štyria v septembri nastúpili na doktorandské štúdium na PriF UK v študijných programoch 4.1.15 Anorganická chémia a 4.1.11 Chemická fyzika. Vzhľadom na zdĺhavú procedúru súvisiacu s udelením vstupných víz, resp. s udelením prechodného pobytu, nástup piateho úspešného uchádzača sa predpokladá začiatkom roka 2020.

V akademickom roku 2018/2019 úspešne ukončil III. stupeň vysokoškolského vzdelania Ing. Michal Slaný v študijnom odbore 5.2.19 Anorganické technológie a materiály akreditovanom na FChPT STU.

Dňa 2.10. 2019 sa konala na ÚACH SAV Súťaž mladých vedeckých pracovníkov do 35 rokov za účasti 12 doktorandov a mladých vedeckých pracovníkov z ÚACH SAV Bratislava a Tn AD Trenčín. Na prvých troch miestach sa umiestnili:

- Florian Lemken
- Tímea Baranyaiová
- Ivana Parchovianská

Špeciálna cena, finančná podpora pre účasť na konferenciu, bola udelená aj Debore Pastvovej, ako PhD študentke v prvom ročníku. Táto cena sa udeľovala po prvý krát, na návrh riaditeľa a bola určená pre súťažiacich z radov začínajúcich PhD. študentov. Zohľadňovala sa vedecká úroveň prezentácie a prejav prednášajúceho.

Do pedagogických aktivít je možné zahrnúť aj pobyt PhD. študentky Eleni Gianni z University of Patras, Grécko v rámci 3-mesačnej stáže financovanej zo SAIA. Eva Scholtzová zaúčala študentku s prácou v programe VASP.

4. Medzinárodná vedecká spolupráca

4.1. Medzinárodné vedecké podujatia

4.1.1. Medzinárodné vedecké podujatia, ktoré organizácia SAV organizovala v roku 2019 alebo sa na ich organizácii podieľala, s vyhodnotením vedeckého a spoločenského prínosu podujatia

XIIth Workshop on Modern Methods in Quantum Chemistry, Mariapfarr, Rakúsko, 45 účastníkov, 11.03.-15.03.2019, 21 prednášok, posterová sekcia, 45 účastníkov (Nemecko, Slovensko, Česká republika, Nórsko, USA, Švajčiarsko)

Engineering Ceramics 2019 – Ceramics for People, Smolenice, Slovensko, 86 účastníkov, 12.05.-16.05.2019

Príprava a vlastnosti progresívnych keramických materiálov a skiel, Ráztočno, 46 účastníkov, 20.11.-22.11.2019

Odborný seminár vedeckých pracovníkov 6 inštitúcií (UACH SAV Bratislava, UMV SAV Košice, VILA Trenčín, FCHPT STU Bratislava, MUNI Brno, CEITEC Brno) s cieľom prezentácie aktuálnych vedeckých výsledkov a nadviazania spolupráce medzi pracoviskami. Na odbornom seminári odznelo 30 prednášok.

4.1.2. Medzinárodné vedecké podujatia, ktoré usporiada organizácia SAV v roku 2020 (anglický a slovenský názov podujatia, miesto a termín konania, meno, telefónne číslo a e-mail zodpovedného pracovníka)

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	3	0	0
Galusek Dušan	1	1	0
Hanzel Ondrej	0	0	1
Hnatko Miroslav	0	0	1
Madejová Jana	1	0	0
Malkin Vladimír	0	0	1
Tatarko Peter	3	0	0
Spolu	8	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

Mgr. Silvia Belušáková, PhD.

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

doc. Ing. Miroslav Boča, DrSc.

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

Mgr. Peter Boháč, PhD.

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

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)

European Society on Glass Science and Technology (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 Lenčéš, 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.

Česká sklárská společnost (funkcia: člen výboru)

Society of Glass Technology (funkcia: člen)

RNDr. Jana Madejová, DrSc.

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

The Clay Minerals Society (funkcia: člen)

Dr. Vladimír Malkin, DrSc.

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

MSc. Daniel Moreno

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

prof. RNDr. Jozef Noga, DrSc.

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

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

Ing. Helena Pálková, PhD.

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

Ing. 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: prezident)

International Ceramic Federation (funkcia: člen predstavenstva)

Materials Research Society (funkcia: člen)

Permanent Executive Committee ECerS (funkcia: volený člen)
World Academy of Ceramics (funkcia: volený člen)

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
Tatarko Peter	Science Fund of the Republic of Serbia / Program PROMIS	4
Lenčes Zoltán	Medzinárodné projekty	1

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

Miroslav Boča

- School of Metallurgy, Northeastern University, Shenyang, Čína, návšteva pracoviska sa uskutočnila na základe pozvania čínskej strany. Predmetom návštevy bola séria prednášok (28 hod.) pre študentov z oblasti spektroskopie, 07. – 30. 10. 2019

Ondrej Hanzel

- Ústav fyziky materiálov, AVČR, Brno, Česká republika (21.10-25.10.2019 a 25.11-27.11.2018). Spoločný projekt, medziakademická spolupráca MAD SAV-AVČR-18-12 „Vývoj nových pokročilých keramických kompozitov pre vesmírne aplikácie“.
- Vinča Institute for Nuclear Science, Belgrade University, Belgrade, Srbsko, spoločný projekt APVV-SK-SRB-18-0022 Ultra-high temperature carbides for extreme environment, 27. - 29.10. 2019

M. Korenko

- School of Metallurgy, Northeastern University (NEU), Čína, spoločný projekt Molten fluorides for metals electrowinning, Medziakademická spolupráca medzi Ústavom anorganickej chémie SAV a NEU, 02. – 13. 09. 2019
- Seaborg Technologies (ST), Kodaň, Dánsko, pozvanie spoločnosti ST na prediskutovanie možnej spolupráce v oblasti fluoridových tavenín pre kompaktný jadrový reaktor na báze roztavených solí vyvíjaný v ST, 28. -29. 08. 2019

B. Kubíková

- School of Metallurgy, Northeastern University, Shenyang, Čína, návšteva pracoviska sa uskutočnila na základe pozvania čínskej strany. Predmetom návštevy boli prednášky pre vybranú skupinu študentov z oblasti termickej analýzy kondenzovaných sústav a fyzikálnochemických vlastností roztavených solí, 07. – 13. 10. 2019

A. Prnová

- University of Gent, Belgicko, spoločný projekt Agreement on scientific cooperation – preparation of amorphous and polycrystalline materials (bulk and thin films) in the systems Al₂O₃-La₂O₃ and Al₂O₃-La₂O₃-ZrO₂. Medziakademická spolupráca MAD medzi Ústavom anorganickej chémie SAV a Univerzitou v Gente, 10. - 24. 11. 2019

M. Micháľková

- CEITEC - BUT, Brno University of Technology, Purkynova 123, Brno, Česká republika, spolupráca SAV VILA a CEITEC, projekt VEGA Transparentné polykrystalické keramické materiály so submikrónovou mikroštruktúrou a luminiscenčnými vlastnosťami, 04. - 09. 08. 2019

Peter Tatarko

- Ústav fyziky materiálů, AVČR, Brno, Česká republika (21.10-25.10.2019 a 25.11-27.11.2018). Spoločný projekt, medziakademická spolupráca MAD SAV-AVČR-18-12 „Vývoj nových pokročilých keramických kompozitov pre vesmírne aplikácie“.
- Ningbo Institute of Materials Technology and Engineering (NIMTE), Chinese Academy of Sciences, Ningbo, Čína, v rámci bilaterálneho projektu APVV-SK-CN-17-0040 Joining of advanced SiC-based ceramic materials, 06.11.-12.11.2019
- Vinča Institute for Nuclear Science, Belgrade University, Belgrade, Srbsko, spoločný projekt APVV-SK-SRB-18-0022 Ultra-high temperature carbides for extreme environment, 27. - 29. 10. 2019

Dlhodobé pobyty na zahraničných inštitúciách (3 mesiace a viac)**M. Barlog**

- International Center for Materials Nanoarchitectonics (WPI-MANA) at the National Institute for Materials Science (NIMS), 14. 07 – 15. 10. 2019, štipendium pre PhD. študentov v rámci NIMS Internship Program.

Peter Boháč

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

Prednášky zahraničných hostí na ÚACH SAV v roku 2019

Dr. Sergey Kuznetsov (Prokhorov General Physics Institute of the Russian Academy of Sciences, Rusko), **06. 08. 2018**

- Inorganic nanofluorides
- Synthesis and spectral-kinetic properties of potential down-conversion materials for solar cells based on Ba₄Y₃F₁₇, GdF₃ and YF₃, CaF₂, SrF₂, doped with Pr³⁺, Ce³⁺, Eu³⁺ and Yb³⁺ ions
- Estimation of Sc³⁺ Solubility in Dodecahedral and Octahedral Sites in Y₃Al₅O₁₂:Yb. Influence of the precursor powder morphology and forming conditions on the high optical transmittance of YAG:Yb ceramics

Dr. Rer. Nat. Branko Matovic (Institute of Nuclear Sciences Vinča, University of Belgrade, Srbsko, **11. 12. 2019**)

- Synthesis of nanometric materials using “Ouzo effect”

Dr. Rer. Nat. Dejan Zagorac (Institute of Nuclear Sciences Vinča, University of Belgrade, Srbsko) **11.12.2019**

- Materials under extreme conditions: From theory to the experiment

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)

Uvádzame 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 vidno 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 2019

Diskusia o akčnom pláne ústavu považuje za obojstranný problém. Navyše 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 zadefinované ciele a ukazovatele zo strany ústavu na strane druhej očakávame aj aktivity zo strany P SAV na podnety zo strany 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.

Akčný plán ÚACH bol vypracovaný k 1.10.2017. Prvý komentár a úpravy boli k 1.2.2019. Následný komentár plánujeme k 31.12.2020; skorší termín nemá opodstatnenie.

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

Sídlo spoločného pracoviska (ak je vytvorené):

Začiatok spolupráce: 1990

Zhodnotenie: Na základe dodatku k zmluve o zriadení spoločného pracoviska je FChPT od roku 2008 členom konzorcia a spoluzriaďovateľom spoločného pracoviska, Centra kompetencie skla Vitrum Laugaricio – VILA. Pracovníci ÚACH viedli na FChPT v roku 2019 troch doktorandov.

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” a „Chemická fyzika”. Spoločne sa riešia projekty VEGA a APVV. Prof. RNDr. J. Noga, DrSc. a prof. RNDr. J. Bujdák, DrSc. majú 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 PríF UK. Pracovníci ÚACH viedli na PríF UK v roku 2019 siedmych doktorandov.

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

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

Sídlo spoločného pracoviska (ak je vytvorené):

Začiatok spolupráce: 1997

Zhodnotenie: Okrem spoločného pracoviska s TnU AD (Centrum kompetencie skla Vitrum Laugaritio) riešil ÚACH SAV v roku 2018 v spolupráci s touto univerzitou 3 spoločné VEGA a dva spoločné APVV projekty. Prof. Ing. P. Galusek, DrSc. prorektor pre vedu, výskum a medzinárodné vzťahy TnU AD je aj členom Vedeckej rady TnU AD a dvoch jej fakúlt (Fakulty zdravotníctva a Fakulty špeciálnej techniky). Pracovníci centra, zamestnanci ÚACH, sa podieľajú na pedagogickej činnosti v rámci vysokoškolského štúdia v odbore "Chemické technológie" a doktorandského štúdia v odbore "Anorganická technológia". V roku 2019 podpísal 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. Skúmanie vlastností takto pripravených materiálov a spoločné publikácie. Na základe dohody o spolupráci prišla Dr. Anna Kityk cez Národný štipendijný program.

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 $\text{Al}_2\text{O}_3\text{-La}_2\text{O}_3$, $\text{Al}_2\text{O}_3\text{-La}_2\text{O}_3\text{-ZrO}_2$, $\text{Al}_2\text{O}_3\text{-Y}_2\text{O}_3$. Skúmanie vlastností pripravených materiálov a spoločné publikácie. MAJEROVÁ, Melinda – PRNOVÁ, Anna – PLŠKO, Alfonz – HRUŠKA, B. – VALÚCHOVÁ, Jana – KRAKNER, J. – BRUNEEL, E. – GALUSEK, Dušan. Crystallization kinetics of Ni-doped $\text{Ca}_2\text{Al}_2\text{SiO}_7$ glass microspheres. In CEEC-TAC5 & Medicta2019. 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry (CEEC-TAC5) and 14th Mediterranean Conference on Calorimetry and Thermal Analysis (Medicta2019): book of abstracts. – Germany: Central and Eastern European Committee for Thermal Analysis and Calorimetry, 2019, p. 479. ISBN 978-3-940237-59-0. (CEEC-TAC5 & MEDICTA 2019 : 5th Central and Eastern Eu

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 FMMI VŠB; doc. Ing. Z. Lenčoš, PhD. je členom odborovej rady doktorandského študijného programu Materiálové vedy a inžinierstvo. Doc. Ing. Miroslav Hnatko, PhD. je školiteľom špecialistom doktoranda z danej fakulty.

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

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

Názov inštitúcie: VÚNAR, a.s.

Oblasť spolupráce: vedecká spolupráca

Sídlo spoločného pracoviska (ak je vytvorené): Nové Zámky

Začiatok spolupráce: 2018

Zhodnotenie: Podaný spoločný projekt vo výzve OPVaI/DP/2018/1.2.1-05

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 praxi

7.2. Kontraktový – zmluvný výskum (vrátane zahraničných kontraktov)

Názov/účel kontraktového výskumu: Výskum a vývoj pokročilých žiaruvzdorných materiálov na báze Al-Si-O-C-N a Zr-O-C-N

Zadávateľ výskumného kontraktu: RHI AG Leoben, Rakúsko

Začiatok spolupráce: 2017

Ukončenie spolupráce: trvá

Finančný prínos pre organizáciu (€): 4700

Názov/účel kontraktového výskumu: Vývoj transparentnej keramiky a iných materiálov

Zadávateľ výskumného kontraktu: CEIT a.s.

Začiatok spolupráce: 2017

Ukončenie spolupráce: trvá

Finančný prínos pre organizáciu (€): 0

Názov/účel kontraktového výskumu: Mapping of the key alumina characteristics for optimal dissolution performance

Zadávateľ výskumného kontraktu: ALUMINIUM PECHINEY, Francúzsko a Hydro Aluminium AS, Nórsko

Začiatok spolupráce: 2018

Ukončenie spolupráce: 2019

Finančný prínos pre organizáciu (€): 120000

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
Mgr. Stanislav Kedžuch, PhD.	Slovenská komisia chemickej olympiády	podpredseda
Ing. Michal Korenko, PhD.	Komisia pre námietky pri verejnom obstarávaní	externý člen
RNDr. Jana Madejová, DrSc.	Komisia pre obhajoby doktorských dizertačných prác v odbore anorganická chémia - 01402	predseda
prof. RNDr. Jozef Noga, DrSc.	Akreditačná komisia SR	člen pracovnej skupiny pre oblasť výskumu Chémia, chemická technológia a biotechnológie
prof. RNDr. Pavol Šajgalík, DrSc.	Rada vlády pre vedu, techniku a inovácie	podpredseda
	Výskumná agentúra SR	člen
	Pandemická komisia MZ SR	člen
	Slovenská komisia pre vedecké hodnosti (SKVH)	podpredseda
	Rada predsedov pracovných skupín pre prioritné oblasti aplikovaného výskumu a experimentálneho vývoja	predseda
	Komisia MŠ pre prioritné oblasti aplikovaného výskumu a experimentálneho vývoja v SR - materiálový výskum a nanotechnológie	člen pracovnej skupiny
	Technologická agentúra SR	člen
	Komisia ministra školstva pre udeľovanie Ceny ministra školstva	člen

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

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
-----------------	--------------	---------

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

9. Vedecko-organizačné a popularizačné aktivity

9.1. Vedecko-popularizačná činnosť

Tabuľka 9a Súhrnné počty vedecko-popularizačných činností organizácie SAV

Typ	Počet	Typ	Počet	Typ	Počet
prednášky/besedy	5	tlač	1	TV	0
rozhlas	1	internet	0	exkurzie	2
publikácie	0	multimediálne nosiče	0	dokumentárne filmy	0
iné	0				

9.2. Vedecko-organizačná činnosť

Tabuľka 9b Vedecko-organizačná činnosť

Názov podujatia	Domáca/ medzinárodná	Miesto	Dátum konania	Počet účastníkov
6. Seminár Slovenskej ílovej spoločnosti: Ílové minerály a vybrané nerudné suroviny v materiálovom výskume, priemyselných aplikáciách a životnom prostredí.	domáca	Banská Bystrica	27.05.-28.05.2019	18
XIIth Workshop on Modern Methods in Quantum Chemistry	medzinárodná	Mariapfarr, Rakúsko	11.03.-15.03.2019	45
Engineering Ceramics 2019 – Ceramics for People	medzinárodná	Smolenice, Slovensko	12.05.-16.05.2019	86
Príprava a vlastnosti progresívnych keramických materiálov a skiel	medzinárodná	Ráztočno	20.11.-22.11.2019	46

9.3. Účasť na výstavách

Názov výstavy: Víkend so SAV

Miesto konania: Primaciálne námestie v Bratislave

Dátum: 21.6.2019

Zhodnotenie účasti:

Na podujatí sa podieľali: Silvia Belušáková, Martin Barlog, Patrícia Petrisková, Michal Slaný, Michal Hičák a Viliam Pavlík.

Všetci fanúšikovia vedy a výskumu si mohli vyskúšať experimenty, súťaže a vedomostné kvízy z rôznych oblastí prírodných a technických vied a spoločenskovedných oblastí. Pripravené boli aj odmeny a darčeky pre deti a mládež. Návštevníci mohli vidieť skutočný meteorit, magnetický vláčik, robotickú hovoriacu hlavu, atrakcie z oblasti chémie, botaniky, biológie, elektrotechniky a informatiky. Vedci predstavili vzácne archeologické a geologické nálezy. Tejto príjemnej akcie sa zúčastnili aj zamestnanci Ústavu anorganickej chémie, ktorí ponúkli návštevníkom zaujímavosti zo sveta anorganických materiálov ako sú keramika, biokeramika, ílové minerály a podobne. Podujatie vo forme popularizačného vedeckého festivalu ponúkol aj takzvanú Živú knihu. Boli to vystúpenia, prednášky a diskusie odborníkov zo SAV pre verejnosť na pripravenom pódiu.

Názov výstavy: Európska noc výskumníkov 2019

Miesto konania: Stará tržnica, Námestie SNP 484, 811 01 Bratislava–Staré Mesto

Dátum: 27.9.2019

Zhodnotenie účasti:

Za ÚACH SAV sa na podujatí podieľali: Martin Barlog, Patrícia Petrisková, Michal Slaný, Michal Hičák, Peter Škorňa, Peter Boháč, Florian Lemken, Daniel Moreno, Debora Pastvová, Marek Pribus, Hakan Ünsal. Európska noc výskumníkov patrí na Slovensku medzi najvýznamnejšie vedecké a popularizačné podujatie. Mladí vedci z ÚACH prezentovali svoju vedecko-výskumnú činnosť širokej verejnosti. Ako fungujú LED diódy a na čo všetko sa používajú keramické materiály v 21. storočí sa mohli účastníci dozvedieť v stánku ÚACH. Účastníci mohli vidieť ukážku rôznych vybraných kovových materiálov, vrátane superzliatin, po vystavení vysokokorozívnemu fluoridovému prostrediu v porovnaní s pôvodnými materiálmi. To, že vrstevnaté silikáty predstavujú materiály s výnimočnými vlastnosťami vedeli už v staroveku. Prečo tomu je tak, a prečo si stále nachádzajú uplatnenie aj v materiáloch 21. storočia sa mohli účastníci dozvedieť vďaka zaujímavým experimentom. Akcia bola zameraná hlavne pre deti v školskom veku, s dôrazom na zvýšenie ich záujmu o štúdium prírodných vied a technických smerov na vysokých školách.

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
Madejová Jana	1	0	0
Pálková Helena	0	0	1
Spolu	1	0	1

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)

New Journal of Glass and Ceramics (funkcia: člen)

doc. Ing. Zoltán Lenčéš, PhD.

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

prof. Ing. Marek Liška, DrSc.

Ceramics - Silikáty (funkcia: člen)

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

International Journal of Applied Glass Science (funkcia: člen)

Sklár a keramik (funkcia: člen)

RNDr. Jana Madejová, DrSc.

Clays and Clay Minerals (funkcia: associate editor)

prof. RNDr. Pavol Šajgalík, DrSc.

Ceramics-Silikáty (funkcia: člen)

Journal of Asian Ceramic Society (funkcia: spolueditor)

Journal of Ceramic Science and Technology (funkcia: člen)

Keramický Zpravodaj (funkcia: člen)

Processing and Application of Ceramics (funkcia: člen)

9.6. Činnosť v domácich vedeckých spoločnostiach

Mgr. Silvia Belušáková, PhD.

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

doc. Ing. Miroslav Boča, DrSc.

Humboldtov klub v SR (funkcia: člen)
Slovenská chemická spoločnosť (funkcia: člen)

Mgr. Peter Boháč, PhD.

Slovenská ílová spoločnosť (funkcia: člen)

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: člen predstavenstva, vedecký tajomník)

Ing. Ondrej Hanzel, PhD.

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)

doc. Ing. Miroslav Hnatko, PhD.

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

doc. Ing. Mária Chromčíková, PhD.

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

Mgr. Ľuboš Jankovič, PhD.

Slovenská ílová spoločnosť (funkcia: člen)

Mgr. Stanislav Kedžuch, PhD.

Slovenská chemická spoločnosť (funkcia: člen predsedníctva)

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.

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská sklárska spoločnosť (funkcia: člen)

RNDr. Jana Madejová, DrSc.

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská ílová spoločnosť (funkcia: podpredseda)

Učená spoločnosť SAV (funkcia: člen)

Ing. Jarmila Mlynáriková, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

MSc. Daniel Moreno

Slovenská ílová spoločnosť (funkcia: člen)

Ing. Zuzana Netriová, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

prof. RNDr. Jozef Noga, DrSc.

Humboldtov klub v SR (funkcia: člen)

Slovenská akademická spoločnosť (funkcia: podpredseda)

Učená spoločnosť SAV (funkcia: predseda)

Ing. Helena Pálková, PhD.

Slovenská ílová spoločnosť (funkcia: člen výboru)

Ing. Viliam Pavlík, PhD.

Slovenská chemická spoločnosť (funkcia: člen)

Ing. Anna Prnová, PhD.

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)

Slovenská Sklárska spoločnosť (funkcia: člen)

Ing. Jaroslav Sedláček, PhD.

Slovenská silikátová vedecko-technická spoločnosť (funkcia: člen)

Ing. Eva Scholtzová, CSc.

Slovenská chemická spoločnosť (funkcia: člen)

Slovenská ílová spoločnosť (funkcia: člen)

Ing. Michal Slaný, 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)

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

Nájdí v sebe vedca:

Začiatkom apríla sa pod taktovkou občianskeho združenia All4Science konala populárno-náučná akcia **Nájdí v sebe vedca** zameraná na školákov piateho až ôsmeho ročníka zo ZŠ Pavla Marceľho na Drieňovej 16 z Bratislavy. Žiaci ôsmeho ročníka navštívili Chemický ústav SAV, ktorý sa do tohto projektu zapája každoročne, a Ústav anorganickej chémie SAV, ktorý žiakov na svoje pôde privítal prvýkrát. Cieľom akcie bolo poukázať na vedu a vedcov z pohľadu súčasnosti, k čomu poslúžila úvodná prednáška prezentovaná interaktívnou formou. Žiaci dostali otázku, ako vyzerá všedný deň vedca. Odpovede boli naozaj variabilné a prednášatelia sa so žiakmi nakoniec hravou formou prepracovali k objasneniu, čo vedec na ústave naozaj robí. Ich záujem počas vysvetľovania stúpol natoľko, že prednášateľov nakoniec zahrnuli všemožnými otázkami z bežného života, napríklad či je mikrovlnka naozaj škodlivá, či máme radšej používať prírodné šampóny alebo prečo stromy rastú.

S jasnou predstavou sa po chvíli ôsmaci odobrali do laboratórií Ústavu anorganickej chémie, kde sa dozvedeli zopár zaujímavých faktov o horení kovov spolu s názornými ukážkami. Ženská časť publika rozmyšľala praktickejšie a ich nechty sa o chvíľu leskli práškovým hliníkom. Potom, ako sa ich oči rozblbli príliš hravými ohníkmi a predstavami o výbuchoch, sa všetci prišli schladiť k experimentom s tekutým dusíkom. Žiaci si mohli beztrešne rozbiť kus vyradeného zamrznutého chemického plášt'a alebo starej chemickej hadice. Poučili ich tiež o osmotickom zákone a o zákone energie chemickej väzby. Najzaujímavejší bol pre nich tzv. Leidenfrostov efekt, ktorý si tí, ktorí sa nebáli, mohli vyskúšať na vlastnej koži. Všetko sa, samozrejme, odohrávalo pod dohľadom zodpovedného pracovníka. A keď už dusíka mali dosť, pozreli sa na záver na farebné spektrum vydávaného pripravenými roztokmi. Fascinujúca paleta farieb bola dosiahnutá absorpciou a premenou ultrafialového svetla na viditeľné žiarenie cez rôzne koncentrácie rodamínových farbív v anorganických emulziách montmorillonitu, ktoré prirovnávali k farbám dúhy. Na záver akcie odchádzali žiaci nadšení z experimentov aj rôznych zaujímavých informácií.

Letná škola mladých vedcov

Sedemnást' detí si v dňoch 22. až 26. júla 2019 mohlo vyskúšať aké je to byť vedcom na **letnom vedeckom tábore**, ktorý pripravili Ústav materiálov a mechaniky strojov a Ústav polymérov SAV v Bratislave. Každý deň bol plný dobrodružstva. Okrem rôznych hier a zábavy, pracovali malí vedci tímovo aj na vlastných projektoch a spoznávali Ústavy SAV. Rozdelení do skupín, si vybrali jeden zo živlov, ktorému sa potom venovali celý týždeň. Na výber mali slnko, vodu a vzduch. V nasledujúce dni skupina SLNKO pracovala na slnečných hodinách, na lome svetla v rôznych prostrediach a na zákonitostiach optiky. V skupine VODA sa pracovalo na blahodarných kozmetických prípravkoch do kúpeľa, na neviditeľnom atramente a na výrobe ekologickej lávovej lampy. Skupina VZDUCH sa pozrela na zúbok reakciám vzduchu v závislosti na teplote a tiež si malí vedci zasimulovali prácu pľúc.

Na nudu nebola príležitosť, pretože ďalší vedecký program bol bohatý a akčný aj vďaka Dr. Viliamovi Pavlíkovi z Ústavu anorganickej chémie. Na Ústave anorganickej chémie pod vedením Ing. Viliama Pavlíka, PhD., pracovali štyria mladí vedci s rôznymi materiálmi v extrémnych podmienkach. Najskôr nazreli do rôznych laboratórií a spoznali, aké prístroje a pomôcky sa v nich využívajú. Diskusiou na vedecko-popularizačnej úrovni sa dozvedeli o energiách vo vesmíre, svete atómov, hmote aj antihmote. Ďalší deň prišiel čas na experimenty. Zistili, ako vplýva nízka teplota na rôzne materiály, a to pomocou tekutého dusíka, do ktorého ich ponárali. Toto ich inšpirovalo k tomu, aby aj oni sami navrhli nejaké pokusy, ktoré by mohli spolu zrealizovať. Adam si vybral výrobu lávy, Matej si chcel vyrobiť vlastnú zliatinu a všetci sa zhodli, že chcú vyrobiť aj strelný prach. Po toľkých experimentoch sa ani nečudujeme, že na našu otázku, či by chceli niečo zmeniť na priebehu letnej školy, zaznela odpoveď: „Aby bola dlhšia!“

Deň otvorených dverí na ÚAC HSAV

Dňa 07.11.2017 už tradične zorganizoval Ústav anorganickej chémie SAV v rámci Týždňa vedy a techniky na Slovensku „Deň otvorených dverí ÚACH SAV“, na ktorý boli pozvaní študenti stredných ako aj vysokých

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

10. Činnosť knižnično-informačného pracoviska

10.1. Knižničný fond

Tabuľka 10a Knižničný fond

Knižničné jednotky spolu		7616
z toho	knihy a zviazané periodiká	7616
	audiovizuálne dokumenty	
	elektronické dokumenty (vrátane digitálnych)	
	mikroformy	
	iné špeciálne dokumenty - dizertácie, výskumné správy	
	Rukopisy, vzácne tlače	
Počet titulov dochádzajúcich periodík		
z toho zahraničné periodiká		
Ročný prírastok knižničných jednotiek		22
v tom	kúpou	22
	darom	
	výmenou	
	bezodplatným prevodom	
	náhradou	
Úbytky knižničných jednotiek		
Knižničné jednotky spracované automatizovane		

Výraz „v tom“ označuje úplné (vyčerpávajúce) údaje, ktorých súčet sa musí rovnať údaju v riadku „spolu“, čiže nadradenému riadku. Výraz „z toho“ označuje neúplné (výberové) údaje, ktorých súčet sa nemusí rovnať údaju v riadku „spolu“.

10.2. Výpožičky a služby

Tabuľka 10b Výpožičky a služby

Výpožičky spolu (riadok 1)		15
v tom z	prezenčné výpožičky	15
r. 1	absenčné výpožičky	0
v tom z	odborná literatúra pre dospelých	15
r. 1	výpožičky periodík	0
MVS iným knižniciam		
MVS z iných knižníc		
MMVS iným knižniciam		
MMVS z iných knižníc		
Počet vypracovaných bibliografií		
Počet vypracovaných rešerší		58

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 €		

10.5. Iné informácie o knižničnej činnosti

11. Aktivity v orgánoch SAV

11.1. Členstvo vo Výbore Snemu SAV

11.2. Členstvo v Predsedníctve SAV a vo Vedeckej rade SAV

prof. RNDr. Pavol Šajgalík, DrSc. - Predseda SAV
- predseda VR SAV

11.3. Členstvo vo vedeckých kolégiách SAV

doc. Ing. Miroslav Boča, DrSc. - VK SAV pre chemické vedy (člen)

RNDr. Jana Madejová, DrSc. - VK SAV pre chemické vedy (člen)

prof. RNDr. Jozef Noga, DrSc. - VK SAV pre chemické vedy (člen)

prof. RNDr. Pavol Šajgalík, DrSc. - VK SAV pre chemické vedy (člen)

11.4. Členstvo v komisiách SAV

doc. Ing. Miroslav Boča, DrSc. - Komisia SAV pre vyhodnocovanie medzinárodných projektov (člen)

Ing. Michal Korenko, PhD. - Komisia pre hodnotenie grantov doktorandov SAV (člen)

11.5. Členstvo v orgánoch VEGA

doc. Ing. Miroslav Boča, DrSc. - Komisia VEGA č. 3 pre chemické vedy, chemické inžinierstvo a biotechnológie (predseda)

prof. Ing. Dušan Galusek, DrSc. - Komisia VEGA č. 7 pre strojárstvo a príbuzné odbory informačných a komunikačných technológií a materiálové inžinierstvo (člen)

doc. Ing. Zoltán Lenčoš, PhD. - Komisia VEGA č. 7 pre strojárstvo a príbuzné odbory informačných a komunikačných technológií a materiálové inžinierstvo (člen)

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

12. Hospodárenie organizácie

12.1. Výdavky organizácie

Tabuľka 12a Výdavky organizácie (skutočnosť k 31. 12. 2019 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
1. Bežné výdavky	2 221 744	1 523 021	553 867	144 856	69
z toho: mzdy (610)	1 080 448	897 961	132 729	49 758	83
vedecká výchova štipendií (640)	51 189	51 189	0	0	100
poistné a príspevok do poisťovní (620)	380 308	312 309	45 140	22 859	82
tovary a služby (630)	578 530	261 562	244 729	72 239	45
transfery partnerom projektov (640)	131 269	0	131 269	0	0
2. Kapitálové výdavky	186 895	0	0	186 895	0
z toho: obstarávanie kapitálových aktív	186 895	0	0	186 895	0
kapitálové transfery	0	0	0	0	0

12.2. Zdroje financovania organizácie

Tabuľka 12b Zdroje financovania organizácie (skutočnosť k 31. 12. 2019 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
1. kapitola SAV (111)	450 459	0	0	2 825	0
z toho: VEGA	102 712			895	
MVTS výskumné projekty	34 996			1 930	
MVTS podpora					
SASPRO/MOREPRO					
Vydávanie časopisov					
Vedecská výchova (štipendií)	51 189				
OTAS (630)	261 562				
2. ŠF EÚ vr. fin. zo ŠR	9 867		7 312	2 555	
3. medzinárodné grantové projekty	60 717	0	30 601	10 695	0
z toho H2020	60 717		30 601	10 695	
4. iné štátne a verejné zdroje (spolu)	544 000		125 417	42 585	131 269

z toho: APVV	544 000	125 417	42 585	131 269
podpora z kapitoly MŠVVaŠ SR (stimuly)				
5. ostatné zdroje	21 800			
z toho: príjmy z prenájmu				
príjmy z podnikateľskej činnosti				
príjmy z expertnej činnosti a služieb	21 800			

13. Nadácie a fondy pri organizácii SAV

14. Iné významné činnosti organizácie SAV

V roku 2019 na ústave prebehli rozsiahle rekonštrukčné práce, pričom boli kompletne zrekonštruované štyri laboratória spolu s ôsmimi kancelármi. Okrem toho v réžii Ú SAV prebiehala rekonštrukcia rozvodov studenej a teplej vody. Obidve akcie boli náročné ako na čas, tak aj na súvisiace aspekty, napr. administratívne (verejné obstarávanie), v prípade rekonštrukcie rozvodov vody trojnásobné rokovanie s Ú SAV a P SAV. V každom prípade treba oceniť ústretovosť orgánov SAV pri riešení súvisiacich problémov. V blízkej dobe sa plánuje rekonštrukcia odpadov na budove, ktorá už začala v bloku A. 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. Problémy, ktoré vznikali počas prác boli zo strany kompetentných riešené povrchno, narýchlo 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 čaká na vyhodnotenie verejného obstarania zhotoviteľa.

15. Vyznamenania, ocenenia a ceny udelené pracovníkom organizácie v roku 2019

15.1. Domáce ocenenia

15.1.1. Ocenenia SAV

Hanzel Ondrej

Súťaž mladých vedeckých pracovníkov SAV do 35 rokov

Oceňovateľ: Predsedníctvo SAV

Opis: 2. miesto v rámci II. Oddelenia vied SAV

Malkin Oľga

Ocenenia SAV za špičkové publikácie, kategória Nature Index publikácie

Oceňovateľ: Predsedníctvo SAV

Opis: za pracu M. Dračínský, M. Buchta, M. Buděšínský, J. Vacek-Chocholoušová, O. L. Malkina, I. Stará and I. Starý, "Dihydrogen contacts observed by through-space indirect NMR coupling", Chem. Sci. 9 (2018), DOI: 10.1039/C8SC02859A Chem. Sci., 2018,9, 7437-7446

15.1.2. Iné domáce ocenenia

15.2. Medzinárodné ocenenia

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

17. Problémy a podnety pre činnosť SAV

Zásadný problém, ktorý narastá niekoľko rokov a v roku 2019 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 jednotlivej 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. P SAV bolo v riešení problému ústretové a zorganizovalo príslušné školenia ako aj kontakt s firmami, ktoré môžu jednotlivým organizáciám pomôcť pri riešení obrovského počtu problémov. Iným ústretovým krokom zo strany predsedníctva bolo napr. poskytnutie vzorovej pracovnej zmluvy alebo vzorovej smernice o používaní IT technológií. Privítame pokračovanie v tomto trende aj s ďalšími dokumentami, ktoré sú v zásade rovnaké pre všetky inštitúcie SAV a vyžadujú sa od každej z nich. Bude určite lacnejšie, ak takéto dokumenty budú vypracované iba raz pre všetky organizácie oproti situácii, keď si takéto dokumenty/smernice dajú vypracovať organizácie jednotlivo.

Správu o činnosti organizácie SAV spracoval(i):

Ing. Helena Pálková, PhD., 02/59410485

Riaditeľ organizácie SAV

Predseda vedeckej rady

.....
doc. Ing. Miroslav Boča, DrSc.

.....
RNDr. Jana Madejová, DrSc.

Prílohy

Príloha A - Zoznam zamestnancov a doktorandov organizácie k 31.12.2019

Zoznam zamestnancov podľa štruktúry

Meno s titulmi	Úväzok (v %)	Ročný prepočítaný úväzok
Vedúci vedeckí pracovníci DrSc.		
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.	45	0.45
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	0.55
Samostatní vedeckí pracovníci		
1. doc. Ing. Tomáš Bučko, PhD.	25	0.25
2. doc. Ing. Miroslav Hnatko, PhD.	100	1.00
3. doc. Ing. Mária Chromčíková, PhD.	100	1.00
4. Mgr. Ľuboš Jankovič, PhD.	100	1.00
5. Mgr. Stanislav Kedžuch, PhD.	100	0.91
6. Mgr. Stanislav Komorovský, PhD.	100	0.50
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. Helena Pálková, PhD.	100	1.00
11. Ing. Viliam Pavlík, PhD.	100	1.00
12. Ing. Anna Prnová, PhD.	100	1.00
13. Ing. Jaroslav Sedláček, PhD.	100	1.00
14. Ing. Eva Scholtzová, CSc.	100	1.00
15. Ing. František Šimko, PhD.	100	1.00
16. Mgr. Peter Švančárek, PhD.	100	1.00
17. Ing. Peter Tatarko, PhD.	100	1.00
18. Mgr. Monika Tatarková, PhD.	100	1.00
19. Ing. Štefan Varga, CSc.	100	1.00
Vedeckí pracovníci		
1. James Richard Asher, PhD	100	1.00
2. Mgr. Tímea Baranyaiová, PhD.	100	0.33
3. Mgr. Peter Boháč, PhD.	100	0.50
4. Mgr. Roman Bystrický, PhD.	20	0.86
5. Ing. Ondrej Hanzel, PhD.	100	1.00
6. Mgr. Valéria Kureková, PhD.	100	0.10
7. Ing. Monika Micháľková, PhD.	60	0.60
8. Ing. Jarmila Mlynáriková, PhD.	100	1.00
9. Ing. Zuzana Netriová, PhD.	100	1.00
10. Mgr. Marek Pribus, PhD.	100	0.33
11. Ing. Michal Slaný, PhD.	100	0.33
12. Ing. Peter Škorňa, PhD.	100	1.00

13.	Ing. Jana Valúchová, PhD.	100	1.00
14.	Ing. Zuzana Vasková, PhD.	100	0.00
Odborní pracovníci s VŠ vzdelaním (výskumní a vývojoví zamestnanci)			
1.	Ing. Martin Barlog	28	0.18
2.	doc. RNDr. Edmund Dobročka, CSc.	20	0.03
3.	Ing. Eva Hadzimová	100	0.00
4.	Ing. Michal Hičák	55	0.04
5.	Ing. Iveta Macková	100	1.00
6.	Ing. Eva Mikšíková	125	1.25
7.	Ing. Jozef Priščák	100	1.00
8.	MSc. Hakan Ünsal	20	0.20
9.	Mgr. Pavol Weiner	100	1.00
Odborní pracovníci s VŠ vzdelaním (ostatní zamestnanci)			
1.	Rastislav Haška	100	1.00
2.	Ing. Ingrid Hierwegová	5	0.05
3.	Ing. Elena Krippelová	100	0.16
4.	Mgr. Martina Pakanová	100	0.58
5.	Ing. Ján Piško	100	1.00
6.	Ing. Jaroslav Rusnák, PhD.	33	0.33
7.	JUDr. Bc. Marica Slaná	100	1.00
Odborní pracovníci ÚSV			
1.	Miroslav Baďura	20	0.20
2.	Iveta Bouadjenak	100	1.00
3.	Slavomír Daniš	100	1.00
4.	Jaromíra Dankovičová	125	1.25
5.	Jarmila Heinleinová	100	1.00
6.	Miriam Hnatková	100	1.00
7.	Anna Jurová	100	1.00
8.	Zdena Kapišinská	35	0.35
9.	Magdaléna Kňazovičová	53	0.53
10.	Anna Kovárová	100	1.00
11.	Alexandra Dominika Rigáňová	100	0.33
12.	Mária Strempekova	100	1.00
13.	Alexandra Tonkovičová	100	1.00
Ostatní pracovníci			
1.	Margita Hudáková	100	1.00
2.	Anna Jurová	20	0.20
3.	Ing. Iveta Macková	20	0.08
4.	Terézia Pírová	100	1.00

Zoznam zamestnancov, ktorí odišli v priebehu roka

	Meno s titulmi	Dátum odchodu	Ročný prepočítaný úväzok
Vedúci vedeckí pracovníci DrSc.			
1.	prof. RNDr. Jozef Noga, DrSc.	31.3.2019	0.13
Samostatní vedeckí pracovníci			
1.	Mgr. Adriana Czímerová, PhD.	31.5.2019	0.41
Vedeckí pracovníci			
1.	Mgr. Silvia Belušáková, PhD.	14.7.2019	0.58
2.	Dr. Mohamed Radwan	31.3.2019	0.24

Odborní pracovníci s VŠ vzdelaním (výskumní a vývojoví zamestnanci)		
1. Hesham Abdelrehim, Dr.	31.8.2019	0.67
2. Ing. Michal Slaný	31.8.2019	0.67
Odborní pracovníci s VŠ vzdelaním (ostatní zamestnanci)		
1. Mgr. Miroslav Adámek	30.4.2019	0.16
2. Ing. Ján Piško	31.12.2019	1.00
Odborní pracovníci ÚSV		
1. Jaromíra Dankovičová	31.12.2019	1.25
2. Magdaléna Kňazovičová	31.12.2019	0.53

Zoznam doktorandov

Meno s titulmi		Škola/fakulta	Študijný odbor
Interní doktorandi hrazení z prostriedkov SAV			
1. MSc. Ramu Ambati	Univerzita Komenského v Bratislave	4.1.15 anorganická chémia	
2. Ing. Martin Barlog	Slovenská technická univerzita v Bratislave	5.2.19 anorganická technológia a materiály	
3. Ing. Michal Hičák	Prírodovedecká fakulta UK	4.1.15 anorganická chémia	
4. Florian Andreas Lemken	Univerzita Komenského v Bratislave	4.1.11 chemická fyzika	
5. Daniel Moreno Rodriguez	Slovenská technická univerzita v Bratislave	5.2.19 anorganická technológia a materiály	
6. Mgr. Debora Pastvová	Univerzita Komenského v Bratislave	4.1.11 chemická fyzika	
7. Mgr. Patrícia Petrisková	Univerzita Komenského v Bratislave	4.1.15 anorganická chémia	
8. Eva Skoura	Univerzita Komenského v Bratislave	4.1.15 anorganická chémia	
9. MSc. Hakan Ünsal	Univerzita Komenského v Bratislave	4.1.15 anorganická chémia	
Interní doktorandi hrazení z iných zdrojov			
<i>organizácia nemá interných doktorandov hrazených z iných zdrojov</i>			
Externí doktorandi			
<i>organizácia nemá externých doktorandov</i>			

Zoznam zamestnancov prijatých do jedného roka od získania PhD.

Meno s titulmi		Dátum obhajoby	Dátum prijatia	Úväzok (v %)
1. Mgr. Marek Pribus, PhD.		30.8.2019	1.9.2019	100
2. Mgr. Tímea Baranyaiová, PhD.		26.8.2019	1.9.2019	100
3. Ing. Michal Slaný, PhD.		26.8.2019	1.9.2019	100

Zoznam emeritných vedeckých zamestnancov

Meno s titulmi

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*)

Zodpovedný riešiteľ:	Peter Tatarko
Trvanie projektu:	1.1.2018 / 31.12.2020
Evidenčné číslo projektu:	2/0116/17
Organizácia je koordinátorom projektu:	áno
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	1 - Česko: 1
Čerpané financie:	-

Dosiahnuté výsledky:

V súlade s plánom projektu bol druhý rok riešenia venovaný príprave nových vysokoteplotných keramických materiálov na báze ZrB_2 -25vol.% SiC s rôznym obsahom (2, 5, a 10 hm.%) oxidov prvkov vzácnych zemín (Eu_2O_3 , Yb_2O_3 a Lu_2O_3). Hutné materiály boli získané spekaním práškových zmesí za asistencie elektrického prúdu pomocou zariadenia "Direct Hot Press", pri podmienkach 2000°C a tlaku 70MPa. Následne boli študované mechanické vlastnosti materiálov pri izbovej teplote na partnerskej organizácii, ÚFM AVČR v Brne. Prísady oxidov prvkov vzácnych zemín boli pridávané do systému ZrB_2 -SiC za účelom zlepšenia vysokoteplotných vlastností týchto materiálov, t.j. odolnosti proti oxidácii a ablácii. Za najdôležitejší výsledok možno považovať to, že mechanické vlastnosti materiálov ZrB_2 -SiC, akými sú tvrdosť, pevnosť a modul pružnosti boli na rovnakej úrovni aj po pridaní 10 hm.% prísad vzácnych zemín, ktorých mechanické vlastnosti sú výrazne odlišné od vlastností matrice. Lomová húževnatosť materiálov dokonca vzrástla po pridaní prísad oxidov prvkov vzácnych zemín. Vysokoteplotné vlastnosti týchto materiálov budú študované v nasledujúcom roku riešenia projektu.

Medziakademická spolupráca s ÚFM AVČR v Brne bola zároveň orientovaná na štúdium mechanických vlastností (tvrdosť, pevnosť a modul pružnosti) keramických spojov na báze SiC a tiež na prípravu nových keramických pórovitých materiálov na báze $\text{Al}_2\text{O}_3/\text{SiO}_2/\text{CaO}$.

Výstupy:

1. FÜRDÖSOVÁ, Zuzana - ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - TATARKO, Peter. ZrB_2 -SiC ceramics with rare-earth oxide additives. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic: book of extended abstracts. Ed. Jana Valúchová; 2019, p. 57-61. ISBN 978-80-971648-8-1. Typ: AFD
2. FÜRDÖSOVÁ, Zuzana - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - DLOUHÝ, Ivo - TATARKO, Peter. Influence of powder processing route and rare earth additives on the mechanical properties of ZrB_2 -SiC ceramics. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019: abstract book. - Italy, 2019, p. 813. Typ: AFG
3. FÜRDÖSOVÁ, Zuzana - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - DLOUHÝ, Ivo - TATARKO, Peter. Preparation and characterization of ZrB_2 -based ceramics with rare earth oxide additives. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019: book of abstracts, p. 71. ISBN 978-80-971648-7-4. Typ: AFH
4. TATARKO, Peter - ZHOU, Xiaobing - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo. Joining of SiC ceramics with Ti-based alloys by SPS. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic: book of extended abstracts. Ed. Jana Valúchová, p. 68-72. ISBN 978-80-971648-8-1. Typ: AFD
5. TATARKO, Peter - SAUNDERS, Theo G. - GRASSO, Salvatore - CHLUP, Zdeněk - DLOUHÝ, Ivo - REECE, Michael J. Interaction between SiC and $\text{Ti}_6\text{Al}_4\text{V}$ in the SPS - From wetting studies to joining. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019: abstract book. - Italy, 2019, p. 177. Typ: AFG
6. TATARKO, Peter - ZHOU, Xiaobing - GRASSO, Salvatore - DLOUHÝ, Ivo - REECE, Michael J. - FERRARIS, Monica. Electric current assisted solid-state diffusion joining of advanced SiC-based ceramics. In CICC-11: The Eleventh International Conference on High-Performance Ceramics, May 25-29, 2019, Kunming, China: abstract book. - China: The Chinese Ceramic Society, 2019, p. 86. Typ: AFG
7. BERTOLLA, Luca - ŠEVEČEK, Oldřich - DLOUHÝ, Ivo - TATARKO, Peter. Composite $\text{Al}_2\text{O}_3/\text{SiO}_2/\text{CaO}$ foams reinforced with cellulose acetate fibres from cigarette tows. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 :

abstract book. - Italy, 2019, p. 27. Typ: AFG

8. BERTOLLA, Luca - CHLUP, Zdeněk - TATARKO, Peter - HANZEL, Ondrej - ŠEVEČEK, Oldřich - ROUPCOVÁ, Pavla - DLOUHÝ, Ivo. Composite Al₂O₃/SiO₂/CaO foams reinforced with cellulose acetate fibers from cigarette tows. In CICC-11: The Eleventh International Conference on High-Performance Ceramics, May 25-29, 2019, Kunming, China: abstract book. - China: The Chinese Ceramic Society, 2019, p. 345. Typ: AFG

Programy: Bilaterálne - iné

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

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

Dosiahnuté výsledky:

Príprava pórovitých mikro guľčiek na báze systému 45S5 bioskla plameňovou syntézou a optimalizácia jej parametrov.
 2. Tvorba C-S-H gélu a natritu na povrchu konvenčne pripraveného bioskla, ktoré sa následne pri plameňovej syntéze rozkladajú a tým pôsobia ako pórtvorné činidlo.
 3. Verifikácia synergického efektu terapeutických iónov bóru a kobaltu pri angiogenéze v bioskle 45S5.

Publikácie:

1. Kraxner, J., M. Michalek, A. R. Romero, H. Elsayed, E. Bernardo, A. R. Boccaccini and D. Galusek (2019). "Porous bioactive glass microspheres prepared by flame synthesis process." Materials Letters 256: 126625.

3.) Vývoj a charakterizácia nových povlakov na báze sklo/keramika pre vysokoteplotné aplikácie (*Development and characterization of a novel glass/ceramic coating systems for high temperature applications*)

Zodpovedný riešiteľ: Dušan Galusek
Trvanie projektu: 1.1.2018 / 31.12.2019
Evidenčné číslo projektu:
Organizácia je koordinátorom projektu: nie
Koordinátor: Universität Bayreuth
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: -

Dosiahnuté výsledky:

1. Vývoj optimálnej metodiky čistenia oceľových substrátov na zabezpečenie adhézie povlakov k oceľovému substrátu.
 2. Vývoj kompozitnej vrstvy na báze PDC so sklenými a keramickými pasívnymi plnivami s vysokou adhéziou k oceľovému substrátu a vysokou odolnosťou voči oxidácii pri teplotách do 1000 °C.

Publikácie:

I. Petriková, M. Parchovianský, P. Švančárek, M. Lenz leite, G. Motz, D. Galusek, Passive filler loaded polysilazane-derived glass/ceramic coating system applied to AISI 441 stainless steel, part 1: Processing and characterization. Int. J. Appl. Ceram. Technol., 1-12, (2019), DOI: 10.1111/ijac.13417

4.) Spájanie moderných keramických materiálov na báze SiC (*Joining of advanced SiC-based ceramic materials*)

Zodpovedný riešiteľ: Peter Tatarko
Trvanie projektu: 1.1.2018 / 31.12.2019
Evidenčné číslo projektu: SK-CN-2017-0040
Organizácia je áno

koordinátorom projektu:**Koordinátor:** Ústav anorganickej chémie SAV**Počet spoluriešiteľských** 0**inštitúcií:****Čerpané financie:** -

Podpora medzinárodnej spolupráce z národných zdrojov: 4000 €

Dosiahnuté výsledky:

V tomto roku sa riešenie projektu zameralo na štúdium mechanických vlastností pri vysokých teplotách, a to vysokoteplotnej pevnosti spojov a ich odolnosti proti teplotným šokom. Počas riešenia projektu bolo pripravených niekoľko sérií SiC spojov, pričom SiC materiály boli spájané pomocou multifázových medzivrstiev na báze TiC/Ti₃SiC₂, ktoré vznikali "in-situ" reakciami počas spájania, alebo pomocou monolitnej medzivrstvy Ti₃SiC₂. Na základe výsledkov pevnosti spojov pri izbovej teplote boli zvolené spoje s najvyššou pevnosťou, pre ktoré sa skúmala pevnosť za vysokých teplôt a odolnosť proti teplotným šokom do 1000°C. Pevnosť multifázových spojov sa lineárne znižovala s rastúcou teplotou. Na druhej strane odolnosť spojov proti teplotným šokom bola veľmi dobrá, s kritickou hodnotou ΔT na úrovni ~940°C. Výsledky preukázali, že prítomnosť prechodovej vrstvy TiC medzi základným materiálom (SiC) a medzivrstvou Ti₃SiC₂ výrazne zníži zvyškové napätia v oblasti spoja, čo priaznivo vplyva na mechanické vlastnosti materiálov. Spoje vytvorené pomocou monolitnej medzivrstvy Ti₃SiC₂ sa vyznačovali najlepšou pevnosťou za vysokých teplôt, nakoľko pri teplote 1200°C si stále držali 68% ich pôvodnej pevnosti.

Výstupy:

1. TATARKO, Peter - ZHOU, Xiaobing - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo. Joining of SiC ceramics with Ti-based alloys by SPS. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic: book of extended abstracts. Ed. Jana Valúchová, p. 68-72. ISBN 978-80-971648-8-1.
2. TATARKO, Peter - SAUNDERS, Theo G. - GRASSO, Salvatore - CHLUP, Zdeněk - DLOUHÝ, Ivo - REECE, Michael J. Interaction between SiC and Ti₆Al₄V in the SPS - From wetting studies to joining. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019: abstract book. - Italy, 2019, p. 177. Typ: AFG
3. TATARKO, Peter - ZHOU, Xiaobing - GRASSO, Salvatore - DLOUHÝ, Ivo - REECE, Michael J. - FERRARIS, Monica. Electric current assisted solid-state diffusion joining of advanced SiC-based ceramics. In CICC-11: The Eleventh International Conference on High-Performance Ceramics, May 25-29, 2019, Kunming, China: abstract book. - China: The Chinese Ceramic Society, 2019, p. 86. Typ: AFG
4. ZHOU, Xiaobing - TATARKO, Peter - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - HUANG, Z. - HUANG, Q. SiC ceramics joined with an in-situ reaction gradient layer of TiC/Ti₃SiC₂ using electric field-assisted sintering technique. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019: book of abstracts. Eds. Zoltán Lenčoš, Jana Valúchová. - Bratislava, Slovakia: Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 52. ISBN 978-80-971648-7-4. Typ: AFF

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

Zodpovedný riešiteľ: Peter Tatarko**Trvanie projektu:** 1.1.2019 / 31.12.2020**Evidenčné číslo projektu:** SK-SRB-18-0022**Organizácia je** áno**koordinátorom projektu:****Koordinátor:** Ústav anorganickej chémie SAV**Počet spoluriešiteľských** 1 - Srbsko: 1**inštitúcií:****Čerpané financie:** -

Podpora medzinárodnej spolupráce z národných zdrojov: 2153 €

Dosiahnuté výsledky:

V súlade s plánom projektu bol prvý rok riešenia zameraný na prípravu keramických materiálov na báze B₄C-TiB₂ a B₄C-SiC, pre využitie pri aplikáciách pracujúcich v extrémnych podmienkach. Prášky boli syntetizované na partnerskej organizácii v Belehrade v Srbsku, pričom ich zhutnenie prebehlo na ÚACH SAV. V prvom prípade boli finálne materiály pripravené reakčným spekaním práškovej zmesi B₄C-TiO₂ pomocou spekania za asistencie elektrického prúdu. Za najdôležitejší výsledok možno považovať to, že materiály boli pripravené pri nižších teplotách a časoch ako sú bežne uvádzané v literatúre. Počas prípravy materiálov B₄C-SiC bolo preukázané, že hutné materiály možno dosiahnuť optimalizovaným procesom spekania za asistencie elektrického prúdu bez nutnosti použitia ďalších spekacích prísad. V oboch prípadoch tieto nové postupy prípravy predstavujú výrazné zníženie nákladov na výrobu týchto materiálov pre

extrémne podmienky. V nasledujúcom období bude štúdium zamerané na charakterizáciu a vlastnosti týchto karbidických materiálov.

Výstupy:

1. ÜNSAL, Hakan - SHEPA, Ivan - MATOVIC, Branko - HANZEL, Ondrej - MÚDRA, Erika - TATARKO, Peter. Densification of B4C-TiB2 composites by field assisted sintering. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic: book of extended abstracts. Ed. Jana Valúchová, 2019, p. 52-56. ISBN 978-80-971648-8-1. Typ: AFD
2. ÜNSAL, Hakan - SHEPA, Ivan - HANZEL, Ondrej - MÚDRA, Erika - VOJTKO, Marek - DUSZA, Ján - TATARKO, Peter. In situ synthesis and characterization of B4C-TiB2 fibers composites. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019: abstract book. Italy, 2019, p. 701. Typ: AFG
3. ÜNSAL, Hakan - SHEPA, Ivan - HANZEL, Ondrej - MÚDRA, Erika - VOJTKO, Marek - DUSZA, Ján - TATARKO, Peter. The effect of temperature and pressure on the densification behaviour of B4C-TiB2(f) composites. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019: book of abstracts, 2019, p. 85. ISBN 978-80-971648-7-4. Typ: AFH
4. ÜNSAL, Hakan - SHEPA, Ivan - HANZEL, Ondrej - MÚDRA, Erika - DUSZA, Ján - TATARKO, Peter. The effect of field assisted sintering parameters on processing of in-situ formed B4C-TiB2 ceramics. In 13th Conference for Young Scientists in Ceramics, October 16-19: book of abstracts, 2019, p. 102. Typ: AFG

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

Zodpovedný riešiteľ:	Peter Tatarko
Trvanie projektu:	1.11.2017 / 31.10.2020
Evidenčné číslo projektu:	MVTS 41090027
Organizácia je koordinátorom projektu:	áno
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	0
Čerpané financie:	-
	Podpora medzinárodnej spolupráce z národných zdrojov: 24000 €

Dosiahnuté výsledky:

V súlade s plánom projektu, bolo riešenie v tomto roku zamerané na optimalizáciu procesu prípravy súvislých vrstiev na báze ZrB₂-SiC-RE₂O₃ na vyleštený povrch CVD-SiC materiálov. Nakoľko riešenie tohto projektu priamo nadväzuje na riešenie projektu H2020 CeramCom (viď nižšie), cieľom bolo nájsť najvhodnejší spôsob nanášania povlakov metódou „aerosol deposition“ na povrch monolitnej keramiky SiC. Tieto poznatky sú následne prenesené a využité pri príprave daných povlakov na povrch keramických kompozitných materiálov (C_f/SiC). Úspešne sa podarilo pripraviť súvislú vrstvu ZrB₂-SiC s minimálnou pórovitosťou, avšak tvrdosť povlaku a adhézia k povrchu nebola dostatočná. Tieto vlastnosti neboli vylepšené ani následným tepelným spracovaním, resp. žihaním. Preto sa pristúpilo k optimalizácii procesu v zmysle nanosenia vrstvy ZrSi₂-B₄C-C na CVD-SiC, pričom takto pripravený materiál bol žišaný pri teplote 1670°C s cieľom in-situ tvorby požadovaného chemického zloženia ZrB₂-SiC. V ďalšom kroku riešenia projektu dôjde k optimalizácii procesu prípravy povlaku ZrB₂-SiC s prídavkom vzácnej zeme (RE₂O₃).

Súbežne bolo štúdium zamerané aj na prípravu hutných diboridových keramik s prísadami RE₂O₃ za účelom nájdenia najvhodnejšieho chemického zloženia v zmysle dosiahnutia najlepšej odolnosti proti oxidácii a ablácii. Pri vývoji týchto materiálov sa tiež preskúmala možnosť ich texturovania, resp. usporiadania zŕn v jednom smere, za účelom zlepšenia mechanických vlastností v požadovanom smere.

Výstupy:

1. TATARKO, Peter - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - MEDVEĎ Dávid - DLOUHÝ, Ivo - REECE, Michael J. Highly textured and strongly anisotropic TiB2 ceramics prepared using magnetic field alignment (9T), In Journal of the European Ceramic Society, 2019, in press, <https://doi.org/10.1016/j.jeurceramsoc.2019.11.006>. Typ: ADCA
2. FÜRDÖSOVÁ, Zuzana - ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - TATARKO, Peter. ZrB2-SiC ceramics with rare-earth oxide additives. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic: book of extended abstracts. Ed. Jana Valúchová; 2019, p. 57-61. ISBN 978-80-971648-8-1. Typ: AFD
3. TATARKO, Peter - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - REECE, Michael J. Preparation of highly textured TiB2-based ceramics using a strong magnetic field. In Engineering Ceramics 2019,

Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts, 2019, p. 51. ISBN 978-80-971648-7-4. Typ: AFH

4. FÜRDÖSOVÁ, Zuzana - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - DLOUHÝ, Ivo - TATARKO, Peter. Influence of powder processing route and rare earth additives on the mechanical properties of ZrB₂-SiC ceramics. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019: abstract book. - Italy, 2019, p. 813. Typ: AFG

5. FÜRDÖSOVÁ, Zuzana - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - DLOUHÝ, Ivo - TATARKO, Peter. Preparation and characterization of ZrB₂-based ceramics with rare earth oxide additives. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019: book of abstracts, p. 71. ISBN 978-80-971648-7-4. Typ: AFH

Programy: ERANET

7.) Multifunkčné hrubé povlaky keramik-grafén pre perspektívne aplikácie (*Multifunctional ceramic/graphene thick coatings for new emerging applications*)

Zodpovedný riešiteľ: Zoltán Lenčes
Trvanie projektu: 1.1.2018 / 31.12.2020
Evidenčné číslo projektu:
Organizácia je koordinátorom projektu: nie
Koordinátor: Institute for Technical Physics and Materials Science, Centre for Energy Research, Hungarian Academy of Sciences (MTA EK)
Počet spoluriešiteľských inštitúcií: 1 - Nemecko: 1, Maďarsko: 1, Slovensko: 3
Čerpané financie: EU: 11502 €

Dosiahnuté výsledky:

V rámci riešenia projektu boli pripravené kompozitné prášky na báze SiC so špekaciami prísadami Y₂O₃ a Sc₂O₃ a s rôznym prídavkom (1, 5 a 10 hm.%) grafénových nanoplatničiek (GNP) alebo oxidu grafénu (GO) pomocou metódy vymrazovacej granulácie. Následne boli takto pripravené kompozitné prášky spekané metódou rapid hot-pressing (RHP) pri teplote 2000°C použitím tlaku 50 MPa v atmosfére N₂ po dobu 30 minút. Časť vzoriek bola žiňaná pri teplote 1800°C v pretlaku dusíka (3 MPa) po dobu 6 h. Relatívna hustota pripravených vzoriek bola vyššia ako 97 %. Na takto pripravených hutných materiáloch bola vykonaná mikroštruktúrna analýza a boli merané funkčné vlastnosti (konkrétne elektrická vodivosť a tepelná difuzivita) v rovnobežnom a kolmom smere vzhľadom na grafénové vrstvy. Taktiež bol skúmaný vplyv prídavku grafénu a efekt žiňania na funkčné vlastnosti materiálov (elektrická a tepelná vodivosť). Elektrická vodivosť kompozitných materiálov sa zvyšovala s rastúcim obsahom grafénu a bola vyššia v smere rovnobežnom s grafénovými platničkami. Taktiež bol pozorovaný pozitívny efekt žiňania. Najvyššia elektrická vodivosť (11800 S/m) bola dosiahnutá pri vzorke s 10 % grafénu po žiňaní v dusíku. V porovnaní s elektrickou vodivosťou referenčnej vzorky (1700 S/m) bez prídavku grafénu sme dosiahli 7 násobný nárast elektrickej vodivosti. Žiňanie pripravených vzoriek v dusíkovej atmosfére malo výrazne pozitívny vplyv na tepelné vlastnosti týchto materiálov. Najvyššie tepelné vodivosti (~240 W/m·K) boli dosiahnuté v smere rovnobežnom s grafénovými vrstvami pri vzorkách s 1 % GO a 5 % GNP po žiňaní. Tieto výsledky dokazujú, že použitie metód vymrazovacej granulácie, spekania v rapid hot-press a žiňanie vzoriek v dusíkovej atmosfére umožňuje získať kompozitné materiály SiC-grafén s vysokou elektrickou a tepelnou vodivosťou.

V rámci riešenia projektu boli taktiež pripravené kompozitné prášky na báze SiC so špekaciami prísadami Y₂O₃ a Al₂O₃ s rôznym prídavkom grafénových nanoplatničiek (5 a 15 hm.%) pomocou metódy vymrazovacej granulácie. Takto pripravené prášky boli lisované s cieľom pripraviť vrstevnaté materiály s vrstvou SiC bez prídavku grafénu, medzivrstvou s 5 hm.% grafénu a vonkajšou vrstvou s vysokým obsahom grafénu (15 hm.%). Takto pripravené vrstevnaté materiály boli spekané pri teplote 1800°C, pri rôznom zaťažení (30, 40 alebo 50 MPa) vo vákuu po dobu 5 minút. Všetky pripravené vzorky vykazovali vysokú hutnosť (relatívna hustota viac ako 99 %). Na takto pripravených vzorkách bola vykonaná základná mikroštruktúrna analýza (veľkosť častíc SiC matrice, distribúcia a preferovaná orientácia grafénových platničiek). V budúcnosti budeme skúmať súdržnosť vrstiev, základné mechanické vlastnosti (tvrdosť, scratch testy) a funkčné vlastnosti (najmä elektrickú a tepelnú vodivosť) vrstevnatých materiálov na báze SiC-grafén.

Publikácie:

HANZEL, Ondrej - SINGH, Meinam Annebushan - MARLA, Deepak - SEDLÁK, Richard - ŠAJGALÍK, Pavol. Wire electrical discharge machinable SiC with GNPs and GO as the electrically conducting filler. In Journal of the European Ceramic Society, 2019, vol. 39, no. 8, p. 2626-2633. (4.029 - IF2018). ISSN 0955-2219. Typ: ADCA

HANZEL, Ondrej - LENČEŠ, Zoltán - KIM, Young-Wook - FEDOR, Ján - ŠAJGALÍK, Pavol. Highly electrically and thermally conductive silicon carbide-graphene composites with yttria and scandia additives. In Journal of the European Ceramic Society, 2020, vol. 40, p. 241-250.

Akceptovaný článok

KIM, Young-Wook - KULTAYEVA, Shynar - SEDLÁČEK, Jaroslav - HANZEL, Ondrej - TATARKO, Peter - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol. Thermal and electrical properties of additive-free rapidly hot-pressed SiC ceramics. In Journal of the European Ceramic Society, 2020, vol. 40, p. 234-240. Akceptovaný článok

HANZEL, Ondrej - LENČEŠ, Zoltán - KIM, Young-Wook - FEDOR, Ján, ŠAJGALÍK, Pavol. Electrical and thermal conductivity of SiC-graphene composites annealed in nitrogen atmosphere. 10. odborný seminár *Interakcie tavenín s progresívnymi anorganickými materiálmi*, 14-15.10.2019, Hradec nad Moravicí, Česká republika, ed. V. Novák, vydala VŠB-TU Ostrava, 2019, p. 4-10.

Programy: Horizont 2020

8.) New Generation Ultra-High Temperature Ceramic Matrix Composites for Aerospace Industry (New Generation Ultra-High Temperature Ceramic Matrix Composites for Aerospace Industry)

Zodpovedný riešiteľ:	Peter Tatarko
Trvanie projektu:	1.6.2018 / 31.5.2020
Evidenčné číslo projektu:	798651
Organizácia je	áno
koordinátorom projektu:	
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských	0
inštitúcií:	
Čerpané financie:	EÚ: 60717 €

Dosiahnuté výsledky:

Riešenie projektu prebiehalo v súlade s plánom na rok 2019. Hlavná aktivita bola venovaná štúdiu zmačateľnosti komplexných práškových zmesí ($\text{ZrB}_2\text{-B}_4\text{C-RE}_2\text{O}_3$) na povrchu keramických kompozitov s keramickou maticou (CMCs), dodaných firmou Airbus Defence & Space. Cieľom štúdie bolo pochopenie fyzikálno-chemických javov prebiehajúcich počas vývoja vysokoteplotných keramických materiálov s keramickou maticou (UHTCMC). Nakoľko nedošlo k požadovanému nataveniu zliatiny a jej infiltrácii do pórovitej matrice pri použití horeuvedenej komplexnej práškovej zmesi, k optimalizácii procesu sa dospelo dvojkrokovou infiltráciou. Dodané materiály boli najprv infiltrované práškom B_4C pomocou vákuovej infiltrácie. Na takto modifikovaných povrchoch kompozitných materiálov bola potom študovaná zmačateľnosť roztavených zliatin ZrB_2 a $\text{ZrB}_2\text{-RE}_2\text{O}_3$. V tomto prípade došlo k požadovanému roztaveniu zliatiny pri teplote 1670°C , pričom taveniny bola infiltrovaná do pórov kompozitov, kde reagovala s B_4C za vzniku požadovaného chemického zloženia $\text{ZrB}_2\text{-SiC-RE}_2\text{O}_3$. Bolo testovaných niekoľko kompozitov s rôznou pórovitosťou za účelom selekcie materiálu, ktorého pórovitosť zabezpečí tvorbu požadovaného chemického zloženia, a rovnomernú infiltráciu zliatiny až do hĺbky cca $800\text{ }\mu\text{m}$. V ďalšom, poslednom roku riešenia projektu budú aktivity venované smerom k tvorbe finálneho povlaku na báze $\text{ZrB}_2\text{-SiC-RE}_2\text{O}_3$ na SiC kompozitoch spevnených uhlíkovými vláknami (C/SiC).

Výstupy:

1. FÜRDÖSOVÁ, Zuzana - ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - TATARKO, Peter. $\text{ZrB}_2\text{-SiC}$ ceramics with rare-earth oxide additives. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic: book of extended abstracts. Ed. Jana Valúchová; 2019, p. 57-61. ISBN 978-80-971648-8-1. Typ: **AFD**

2. TATARKO, Peter - VALENZA, Fabrizio - ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - BYSTRICKÝ, Roman. Wetting and phase interaction between C/SiC and transition metal disilicides-based alloys. In HT-CMC10. 10th International conference on high temperature ceramic matrix composites, September 22-26, 2019, Bordeaux, France: book of abstracts. - France, 2019, p. 323. Typ: **AFG**

Domáce projekty

Programy: VEGA

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

Zodpovedný riešiteľ: Miroslav Boča
Trvanie projektu: 1.1.2016 / 31.12.2019
Evidenčné číslo projektu: 2/0114/16
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 17085 €

Dosiahnuté výsledky:

Zlúčenina α -K₂ZrF₆ podlieha nezvyčajnej viacstupňovej modifikačnej premene v tuhom stave. Táto modifikačná premena môže byť reverzibilná alebo ireverzibilná vzhľadom na cieľovú teplotu. Zahrievanie K₂ZrF₆ na 250 °C spôsobuje nevratnú modifikačnú premenu, ktorej produktom je fáza označená ako meta-K₂ZrF₆ a fáza K₃ZrF₇. Starnutie takejto zmesi podlieha ďalšiemu procesu premien, kedy vzniká aj fáza α -K₂ZrF₆ ale nárast jej koncentrácie sa zastaví, keď dosiahne rovnaký podiel ako meta-K₂ZrF₆. V prípade, že α -K₂ZrF₆ je zahriata na teplotu vyššiu ako 250 °C pri chladení nastane reverzibilná premena vysokoteplotnej fázy naspäť na α -K₂ZrF₆ fázu. Proces transformačných premien bol sledovaný rôznymi metódami ako DTA, DSC, ¹⁹F MAS NMR, XRD, tepelnou difúziou a Ramanovou spektroskopiou. Zaujímavosťou je aj to, že odozva monitorovania modifikačných premien rôznymi technikami vykazovala neočakávané rozpory, ktoré bolo treba interpretovať.

Publikácie a príspevky:

BOČA, Miroslav** – NETRIOVÁ, Zuzana – RAKHMATULLIN, Aydar – VASKOVÁ, Zuzana – HADZIMOVÁ, Eva – SMRČOK, Ľubomír – HANZEL, Ondrej – KUBÍKOVÁ, Blanka. The differing responses of various techniques in measuring the phase transformations of K₂ZrF₆. In Journal of Molecular Liquids, 2019, vol. 287, p. 110969-110969-10. (4.561 – IF2018). (2019 – Current Contents, WOS, SCOPUS). ISSN 0167-7322. Typ: **ADCA**
 HRUŠKA, Branislav** – NETRIOVÁ, Zuzana – VASKOVÁ, Zuzana – BOČA, Miroslav – CHROMČÍKOVÁ, Mária – LIŠKA, Marek. High-temperature Raman study of K₂ZrF₆ phase transitions. In Journal of Alloys and Compounds, 2019, vol. 791, p. 45-50. (4.175 – IF2018). (2019 – Current Contents, WOS, SCOPUS). ISSN 0925-8388. Typ: **ADCA**
 BOČA, Miroslav – ŠIMURDA, Michal – ŠVEC, Peter – ŠVEC, Peter Jr. – JANIČKOVIČ, Dušan – CZÍMEROVÁ, Adriana – KUBÍKOVÁ, Blanka – MLYNÁRIKOVÁ, Jarmila. Unusual phase transformations in ternary fluoride systems. In 19th European Symposium on Fluorine Chemistry: Book of Abstracts. - Warszawa, Poland: Oficyna Wydawnicza Poligraficzna ADAM, 2019, p. 134. Type: **AFF**
 BOČA, Miroslav – ŠIMURDA, Michal – ŠVEC, Peter – ŠVEC, Peter Jr. – JANIČKOVIČ, Dušan – CZÍMEROVÁ, Adriana – KUBÍKOVÁ, Blanka – MLYNÁRIKOVÁ, Jarmila. Unusual phase transformations in ternary fluoride systems. In MS11. 11th international symposium on molten salts - chemistry and technology, 19-23 Mai 2019, Orleans, France: program and abstracts. - France, 2019, p. 87. Type: **AFG**
 BOČA, Miroslav – ŠIMURDA, Michal – ŠVEC, Peter – ŠVEC, Peter Jr. – JANIČKOVIČ, Dušan – CZÍMEROVÁ, Adriana – KUBÍKOVÁ, Blanka – NETRIOVÁ, Zuzana – MLYNÁRIKOVÁ, Jarmila. Unusual phase transformations in ternary fluoride systems. In ChemZi : Zborník abstraktov: 71. Zjazd chemikov, 9-13 september 2019, Vysoké Tatry, Horný Smokovec, Slovensko. - Bratislava: Slovenská chemická spoločnosť, 2019, roč. 15, č. 1, s. 82. ISSN 1336-7242. Typ: **AFH**

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

Zodpovedný riešiteľ: Adriana Czímerová
Trvanie projektu: 1.1.2017 / 31.05.2019
Evidenčné číslo projektu: 2/0156/17
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: -

Dosiahnuté výsledky:

Projekt bol predčasne ukončený.

3.) Nové anorganické fosfory na báze stechiometrických hlinitanov a kremičitanov s dlhodobou svetelnou emisiou pre optické a biomedicínske aplikácie (*Nové anorganické fosfory na báze stechiometrických hlinitanov a kremičitanov s dlhodobou svetelnou emisiou pre optické a biomedicínske aplikácie*)

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: SAV: 4686 €

Dosiahnuté výsledky:

Pripravené boli luminofory v sústave SrAl_2O_4 dopované Dy^{3+} a kombináciou opticky aktívnych provkov $\text{Dy}^{3+}/\text{Eu}^{2+}$ reakciou v tuhej fáze pri teplotách nad 1300°C v redukčnej atmosfére. Sledoval sa vplyv podmienok prípravy luminoforov a koncentrácie dopantov na dĺžku dosvitu pripraveného luminoforu.

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

Zodpovedný riešiteľ: Dušan Galusek
Trvanie projektu: 1.1.2017 / 31.12.2020
Evidenčné číslo projektu: 2/0026/17
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 6170 €

Dosiahnuté výsledky:

1. Príprava transparentnej MgAl_2O_4 keramiky metódou SPS a optimalizácia podmienok zabráňujúcich kontaminácii materiálu uhlíkom počas spekania.
 2. Otestovanie nových typov prísad na podporu spekania (CoF_2 , MnF_2) pre prípravu vysoko hutnej keramiky na báze MgAl_2O_4 , ktoré zároveň slúžia ako zdroj opticky aktívnych dopantov.
 3. Aplikácia metódy Master Sintering Curve na hodnotenie priebehu spekania spinelovej keramiky.
 Publikácie

1. Ali Talimian, Dusan Galusek; Aqueous slip casting of translucent magnesium aluminate spinel: Effects of dispersant concentration and solid loading; *Ceramics International* 45 (2019) 10646–10653; doi.org/10.1016/j.ceramint.2019.02.134
 2. Talimian Ali - Puchlý V. - El-Maghraby Hesham F. - Maca K. - Galusek Dušan: Impact of high energy ball milling on densification behaviour of magnesium aluminate spinel evaluated by master sintering curve and constant rate of heating approach, In: *Ceramics international*. - ISSN 0272-8842. - Vol.45, No.17(2019), p.23467-23474, part B., <https://doi.org/10.1016/j.ceramint.2019.08.051>

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

Zodpovedný riešiteľ: Miroslav Hnatko
Trvanie projektu: 1.1.2018 / 31.12.2021
Evidenčné číslo projektu: 2/0152/18

Organizácia je áno
koordinátorom projektu:
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 9709 €

Dosiahnuté výsledky:

V súlade s harmonogramom projektu sme na začiatku druhej etapy, zahájili optimalizáciu spôsobu prípravy trabekulárnych telies z SN granúl. Zámerom je vyvinúť technológiu prípravy pórovitého, bioaktívneho, antibakteriálneho skeletu s dostatočnou pevnosťou, ktorá by sa dala využiť pri príprave náhrad kostí rôznych tvarov a veľkostí jednoduchým a rýchlym spôsobom. Úlohou bolo spojiť pripravené granule do pevného skeletu vytvorením „křčkov“ medzi nimi a to rýchlym zahrevom na optimálnu teplotu s krátkou výdržou a rýchlym schladením. Ako bioaktívnu a zároveň spájaciu zložku sme použili štyri rôzne systémy, ktoré boli do granúl primiešané už v procese ich prípravy, alebo neskôr, boli do nich infiltrované vo forme sólu (system CaSiO_3 ; $\text{CaO-P}_2\text{O}_5\text{-SiO}_2$; vodné sklo s vyšším podielom Na_2O ; a Bioglass®.). V rámci charakterizácie kompozitných materiálov na báze kalcium-fosfátových cementov s prídavkom pórovitých SN mikroguličiek bol stanovený súbor fyzikálno-chemických a biologických vlastností týchto materiálov. Výsledky sú spracované do formy publikácie, ktorá je pred zaslaním.

Publikácie:

BYSTRICKÝ, Roman - HNATKO, Miroslav - SEDLÁČEK, Jaroslav. Preparation of lightweight aggregates from industrial waste. In Preparation of ceramic materials: Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. Košice: Technical University, 2019, p. 33-37. ISBN 978-80-553-3314-4.(Preparation of ceramic materials : international conference). AFD
 HIČÁK, Michal - HNATKO, Miroslav - LABUDOVÁ, Martina - GALUSKOVÁ, Dagmar - SEDLÁČEK, Jaroslav - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol. Bioproperties of Si_3N_4 -based ceramics after oxy-acetylene flame treatment = Biologické vlastnosti keramiky na báze Si_3N_4 po opracovaní povrchu kyslíkovo-acetylenovým plameňom. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic: book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Micháľková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic: Institute of Inorganic Chemistry SAS, 2019, p. 30-41. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses). AFD
 HNATKO, Miroslav - HIČÁK, Michal - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Surface modification of dense silicon nitride. In Preparation of ceramic materials: Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. - Košice: Technical University, 2019, p. 103-109. ISBN 978-80-553-3314-4.(Preparation of ceramic materials : international conference). AFD
 TATARKOVÁ, Monika - TATARKO, Peter - DLOUHÝ, Ivo - DUSZA, Ján. Sintering behaviour and microstructural evolution of silicon nitride composites with boron nitride platelets. In Preparation of ceramic materials: Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. Košice: Technical University, 2019, p. 111-114. ISBN 978-80-553-3314-4.

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

Zodpovedný riešiteľ: Mária Chromčíková
Trvanie projektu: 1.1.2018 / 31.12.2021
Evidenčné číslo projektu: 1/0064/18
Organizácia je nie
koordinátorom projektu:
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 2913 €

Dosiahnuté výsledky:

Riešenie sa zameralo na problematiku parametrizácie termodynamických modelov úžitkových skiel. Riešil sa problém chýbajúceho reprezentanta štruktúrnej jednotky Q3 pre binárny subsystem CaO-SiO_2 . Model sa preto rozšíril o zlúčeninu $\text{CaO} \cdot 2\text{SiO}_2$. Navrhla a validovala sa metóda odhadu molárnej Gibbsovej energie tejto zlúčeniny založená na lineárnej závislosti reakčnej Gibbsovej energie na vytvorenie jedného nemostikového kyslíka v štruktúrnej jednotke Qn na hodnote n. Výsledky boli publikované v práci: M. Liška, J. Macháček, M. Chromčíková, R. Svoboda: Thermodynamic model of CaO-SiO_2 glasses. Ceramics-Silikáty, doi: 10.13168/cs.2019.0049

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

Zodpovedný riešiteľ: Mária Chromčíková
Trvanie projektu: 1.1.2016 / 31.12.2020
Evidenčné číslo projektu: 2/0088/16
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 1 - Slovensko: 1
Čerpané financie: SAV: 1751 €

Dosiahnuté výsledky:

Riešenie projektu sa sústredilo na validovanie termodynamických modelov fosforečnanových a boritanových skiel cestou porovnania výsledkov analýzy sérií Ramanových spektier matematicko-štatistickými metódami PCA a MCR s výsledkom rozkladov týchto spektier Malfaitovou metódou založenou rovnovážnych látkových množstvách zložiek termodynamického modelu.

Pre binárne bárnato-fosforečnanové sklá s nízkym obsahom Al_2O_3 sa preskúmala entalpická a štruktúrna relaxácia. Výsledky sa interpretovali v kontexte termodynamického modelu sústavy $\text{BaO-Al}_2\text{O}_3\text{-P}_2\text{O}_5$.

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

Zodpovedný riešiteľ: Zoltán Lenčes
Trvanie projektu: 1.1.2018 / 31.12.2021
Evidenčné číslo projektu: 2/0164/18
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 14893 €

Dosiahnuté výsledky:

Experimentálne boli pripravené luminofoři na báze LaSi_3N_5 dopované Ce, Eu, Sm, Er, Nd a Yb. Luminofoři boli pripravené zo zmesi nitrid-oxid ($\text{LaSi}_3\text{N}_5/\text{Ln}_2\text{O}_3$) a nitrid fluorid ($\text{LaSi}_3\text{N}_5/\text{LnF}_3$) žiahaním pri 1600 °C po dobu 3 h v pretlaku dusíka 2 MPa. Fluoridy majú výrazne nižšiu teplotu topenia v porovnaní s oxidmi, čo umožňuje prípravu luminoforov pri nižších teplotách, čo bolo dokázané aj experimentmi. Teplotu syntézy sme znížili o 150 °C v prípade luminoforov s prídavkom dopantov vo forme fluoridov. Luminofoři dopované fluoridmi vykazujú pomerne ostré/úzke emisné píky s maximom 546 nm pre CeF_3 -dopovaný materiál, pri 397 nm a 468 nm pre ErF_3 a pri 483 nm pre YbF_3 dopovaný LaSi_3N_5 luminofoři. V prípade luminoforov LaSi_3N_5 dopovaných oxidmi lantanoidov boli namerané výrazne širšie emisné píky (pri 510 – 625 nm pre CeO_2 dopovaný materiál, 370 – 600 nm pre Er_2O_3 , a 440 – 600 nm pre Yb_2O_3 dopovaný materiál). Bola stanovená aj doba trvania excitovaných stavov luminoforu, ktorá sa pohybovala v rozmedzí 120 ns ($\text{LaSi}_3\text{N}_5\text{:Ce}$) až 300 ns ($\text{MgSiN}_2\text{:Eu}$). Tieto doby zhasania umožňujú aplikovať vyvinuté luminofoři nielen v LED, ale aj v displejoch s vysokou ostrosťou farieb.

V prípade materiálov na báze $\text{LaSi}_3\text{N}_5\text{:Nd}$ neboli pozorované žiadne emisie vo viditeľnej oblasti spektra. Silné emisie boli namerané v blízko-infračervenej oblasti s maximami pri 895 nm a 1083 nm. Tieto materiály môžu byť použité napr. v infralampách na liečbu IČ svetlom.

V rámci riešenia projektu boli študované aj keramické podložky na báze Si_3N_4 a SiC s vysokou tepelnou vodivosťou a kontrolovanou elektrickou vodivosťou, ktoré by v prípadnej aplikácii vyvinutých luminoforov v LED znížili riziko tepelného zhasania vďaka dobrému odvodu tepla od vrstvy luminoforov zaliatych do živice alebo silikónu. Jedná sa o spoluprácu s Functional Ceramics Laboratory, Department of Materials Science and Engineering, University of Seoul, (prof. Young-Wook Kim)

Podrobnejšie boli študované luminiscenčných vlastností spinelu (MgAl_2O_4) dopovaného Cr^{3+} . Cieľom bolo overiť možnosť náhrady drahých dopantov z radu lantanoidov lacnejšími prechodnými prvkami. Luminofoři $\text{MgAl}_2\text{O}_4\text{:Cr}^{3+}$ vykazoval slabú emisiu s maximom pri 370 nm (fialové svetlo) po excitácii $\lambda_{\text{ex}} = 250$ nm. Po excitácii zeleným svetlom ($\lambda_{\text{ex}} = 500 - 550$ nm) bola nameraná silná emisia v tmavo-červenej oblasti viditeľného svetla s maximom pri 690 – 710 nm.

Študoval sa aj vplyv množstva Eu v koncentračnom rozsahu 0,5 mol% až 3 mol% na luminiscenčné vlastnosti spinelu MgAlON (tuhý roztok MgAl_2O_4 a AlN). Emisné spektrá vzoriek po excitácii 350 nm žiarením mali maximum emisie je pri 472 nm (modré svetlo). Z výsledkov vyplýva, že najvyššia intenzita emitovaného žiarenia bola dosiahnutá v prípade MgAlON vzorky dopovanej 0,5 mol% Eu, potom pri zvyšujúcom sa obsahu Eu dochádzalo ku koncentračnému zhášaniu. V porovnaní so vzorkou $\text{MgAl}_2\text{O}_4\text{:Eu}$ ($\lambda_{\text{em,max}} = 460$ nm) došlo k červenému posuvu maxima v dôsledku prítomnosti dusíka v štruktúre a zvýšeniu kovalentnosti väzieb v blízkom okolí dopantu.

Publikácie:

Young-Wook Kim, Shynar Kultayeva, Jaroslav Sedláček, Ondrej Hanzel, Peter Tatarko, Zoltán Lenčేశ, Pavol Šajgalík: Thermal and electrical properties of additive-free rapidly hot-pressed SiC ceramics. J. Eur. Ceram. Soc., 40 (2020) 234-240.

Y. Duan, J. Zhang, X. Li, H. Bai, P. Šajgalík, D. Jiang, High thermal conductivity silicon nitride ceramics prepared by pressureless sintering with ternary sintering additives. Int. J. Appl. Ceram. Technol., (2019) 1-8. <https://doi.org/10.1111/ijac.13220>

O. Hanzel, M.A. Singh, D. Marla, R. Sedlák, P. Šajgalík, Wire electrical discharge machinable SiC with GNPs and GO as the electrically conductive filler. J. Eur. Ceram. Soc., 39 (2019) 2626-2633. <https://doi.org/10.1016/j.jeurceramsoc.2019.03.012>

O. Hanzel, Z. Lenčేశ, Y.-W. Kim, J. Fedor, P. Šajgalík, High electrically and thermally conductive silicon carbide – graphene composites with yttria and scandia additives. J. Eur. Ceram. Soc., (2019) under review. Manuscript Ref. No.: JECS-D-19-01506

LENČEŠ, Zoltán - RADWAN, Mohamed - ŠAJGALÍK, Pavol. Preparation of transparent MgAl_2O_4 ceramics for LED applications. In ICACC 2019. 43rd International Conference & Exposition on Advanced Ceramics and Composites, January 27 - February 1, 2019, Daytona Beach, Florida, USA: abstract book. USA: The American Ceramic Society, 2019, p. 36. (ICACC 2019. International Conference & Exposition on Advanced Ceramics and Composites). AFG

Z. Lenčేశ, M. Radwan, A. Czimerová, P. Šajgalík, Preparation of transparent/translucent spinel-based phosphors. Abstract Book of the XVIth Conference and Exhibition of the European Ceramic Society, 16-20 June 2019, Torino, Societa Ceramica Italiana, p. 507. AFG

LENČEŠ, Zoltán - CZÍMEROVÁ, Adriana - PETRISKOVÁ, Patrícia - KLEMENT, Róbert - HULMAN, Martin. Influence of lanthanide oxides and fluorides on the photoluminescence of LaSi_3N_5 . In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019: book of abstracts. - Bratislava, Slovakia: Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 79. ISBN 978-80-971648-7-4.

PETRISKOVÁ, Patrícia - RADWAN, Mohamed - MONFORT, O. - PLESCH, Gustáv - LENČEŠ, Zoltán. Photocatalytic TiO_2 nanotubes arrays formation on polymeric and ceramic substrates. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019: book of abstracts. - Bratislava, Slovakia: Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 81. ISBN 978-80-971648-7-4. (Engineering Ceramics 2019: Ceramics for people). AFH

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

Zodpovedný riešiteľ:	Jana Madejová
Trvanie projektu:	1.1.2017 / 31.12.2020
Evidenčné číslo projektu:	2/0141/17
Organizácia je	áno
koordinátorom projektu:	
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských	0
inštitúcií:	
Čerpané financie:	SAV: 17085 €

Dosiahnuté výsledky:

V treťom roku riešenia projektu boli skompletizované interpretácie výsledkov zamerané na sledovanie rôznych faktorov vplyvujúcich na usporiadanie/konformáciu alkylamóniových surfaktantov ako sú dĺžka alkylového reťazca, typ centrálnej skupiny surfaktantu a teplota. Získané výsledky boli publikované v prácach [1, 2]. Pozoroval sa aj vplyv náboja vrstiev troch rôznych montmorillonitov (SAz, JP a SWy) na usporiadanie surfaktantov. Zistilo sa, že so stúpajúcim nábojom vrstiev narastá množstva usporiadaných "trans" a klesá neusporiadaných "gauche" konformérov. Modifikáciou montmorillonitu JP kationmi 4C1-N/P, 4C4-N/P, 4-C8-N/P, 3C8-N/P-1C12, 3C8-N/P-1C14, 3C8-N/P-1C16 sa pripravili dve série organoílov s rôznou veľkosťou organického kationu a rôznym centrálnym atómom (N alebo P). Testovali sa experimentálne podmienky s cieľom získať kompletnú výmenu anorganických Na-kationov za kationy organické. Ab initio molekulová dynamika na DFT úrovni bola použitá na štúdium štruktúry montmorillonitu (Mt) interkalovaného

tetrabutylamóniovým (TBA) a tetrabutylfosfóniovým (TBP) kationom. Analýza medziatómových vzdialeností ukázala, že slabé C–O...H vodíkové väzby sú dôležité pre stabilizáciu oboch kationov, pričom trochu silnejšie H-väzby boli indikované pre TBP kation. Vypočítané interkalačné a adsorpčné energie potvrdili, že TBP-Mt je stabilnejší ako TBA-Mt [3]. V rámci úlohy zameranej na trojzložkové materiály s fotoaktívnymi farbivami sa študovali vlastnosti hybridného nanokompozitného materiálu na báze ílového nosiča smektitu, fluoresceínom modifikovaného polymérneho dextránu (FITC) a fotosenzibilizátora v podobe aniónového farbiva floxín B (PhB). Cieľom bolo pripraviť tenké filmy s vysokoúčinnou absorpciou žiarenia vo viditeľnej oblasti s následným rezonančným prenosom tejto energie z FITC na PhB. Takéto materiály majú potenciálne využitie ako antimikrobiálne fotosenzibilizačné materiály s možnosťou využitia polychromatického žiarenia [4].

V rámci dlhodobej medzinárodnej spolupráce časť experimentov sa zamerala na prípravu pórovitých heteroštruktúrnych materiálov na báze montmorillonitu, tzv. porous clay heterostructures (PCH), ktoré môžu predstavovať zaujímavú alternatívu k rôznym štruktúram na báze SiO₂. Optimalizáciou podmienok syntézy (koncentrácia FeCl₃, ktorý sa použil ako zdroj Fe³⁺, tlak, čas impregnácie a kalcinácie) sa pripravil kompozitný materiál PCH/FeOx s vysokou efektívnosťou v reakcii rozkladu toluénu. Práca poskytla originálne interpretácie zmien IČ spektrách v ďalej oblasti s podporou DFT výpočtov, čím sa potvrdila prítomnosť α -Fe₂O₃ a Fe₃O₄ fáz na povrchu Fe-PCH [5].

[1] SLANÝ, Michal - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana. Structural characterization of organo-montmorillonites prepared from a series of primary alkylamines salts: Mid-IR and near-IR study. In *Applied Clay Science*, 2019, vol. 176, p. 11-20. (3.890 - IF2018).

[2] MADEJOVÁ, Jana - JANKOVIČ, Ľuboš - SLANÝ, Michal - HRONSKÝ, Viktor. Conformation heterogeneity of alkylammonium surfactants self-assembled on montmorillonite: Effect of head-group structure and temperature. In *Applied Surface Science*, 2020, vol. 503, art. no. 144125. (5.155 - IF2018).

[3] SCHOLTZOVÁ, Eva - TUNEGA, Daniel. Density functional theory study of the stability of the tetrabutylphosphonium and tetrabutylammonium montmorillonites. In *Clay Minerals*, 2019, vol. 54, no. 1, p. 41-48. (1.787 - IF2018).

[4] KUREKOVÁ, Valéria - Belušáková, Silvia - Boháč, Peter – Bujdák, Juraj. Resonance energy transfer in the systems of smectite modified with a fluorescent cationic polymer and a photosensitizer. In *Applied Clay Science*, 2019, vol. 183, art. no. (3.890 - IF2018).

[5] ZIMOWSKA, Malgorzata - GURGUL, J. - SCHOLTZOVÁ, Eva - SOCHA, Robert P. - PÁLKOVÁ, Helena - LITYNSKA-DOBRZYNSKA, L. - MORKZYCKI, Lukasz - LATKA, K. A precursor approach for the development of lace-like Fe₂O₃ nanocrystallites triggered by pressure dependent nucleation and growth of akaganeite over clay based composites for toluene combustion. In *Journal of Physical Chemistry C*, 2019, vol. 123, no. 43, p. 26236-26250. (4.309 - IF2018).

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

Zodpovedný riešiteľ:	Oľga Malkin
Trvanie projektu:	1.1.2017 / 31.12.2020
Evidenčné číslo projektu:	2/0116/17
Organizácia je koordinátorom projektu:	áno
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	0
Čerpané financie:	SAV: 13142 €

Dosiahnuté výsledky:

KONEČNÝ, Lukáš** – REPISKÝ, Michal – RUUD, Kenneth – KOMOROVSKÝ, Stanislav**. Relativistic four-component linear damped response TDDFT for electronic absorption and circular dichroism calculations. In *Journal of Chemical Physics*, 2019, vol. 151, no. 19, p. 194112-1-194112-14. (2.997 – IF2018). ISSN 0021-9606. Typ: ADCA

11.) 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: 5914 €

Dosiahnuté výsledky:

V prvom roku projektu sa úspešne pripravili modely špirálovitej štruktúry hallozyitu, planárneho haloyzitu s irinotekanom(liečivo), hektoritu, hybridných komplexov cholin/acetylcholin -beidelit(Bd)/montmorilonit(Mt), atrazín-Bd/Mt a chrómanov v Bd. Štruktúry hybridných komplexov íl-polutant boli pripravené a charakterizované aj experimentálne. Čiastkové výsledky boli prezentované na vedeckých konferenciách formou prednášok a postrov. Všetky výsledky získané v tomto období sa spracúvajú do článkov v renomovaných vedeckých časopisoch.

Výstupy:

SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - ŠKORŇA, Peter - MORENO RODRÍGUEZ, Daniel - TUNEGA, Daniel. Insight into the stability of beidellite intercalates. In BIT's 7th Annual Conference of AnalytiX-2019, April 12-14, 2019, Singapore: conference handbook.Exploring Innovative Advances and Applications. - Singapore, 2019, p. 78.
 SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - ŠKORŇA, Peter - MORENO RODRÍGUEZ, Daniel - TUNEGA, Daniel. Tetraalkylphosphonium beidellite intercalates - structural stability by DFT method. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France: book of abstracts. - Paris, France, 2019, p. 556. (EUROCLAY 2019. International conference on clay science and technology).

MORENO RODRÍGUEZ, Daniel - SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - TUNEGA, Daniel. Atrazine-Montmorillonite/Beidellite intercalates: a density functional theory study. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France: book of abstracts. - Paris, France, 2019, p. 456. (EUROCLAY 2019. International conference on clay science and technology).

ŠKORŇA, Peter - SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - TUNEGA, Daniel. Structural properties and spectroscopic characterization of choline-beidellite and acetylcholine-beidellite intercalates. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France: book of abstracts. - Paris, France, 2019, p. 571.

MORENO RODRÍGUEZ, Daniel - SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - TUNEGA, Daniel. Density functional theory study of atrazine-beidellite intercalates. In 6th Workshop of Slovak Clay Group: Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia: book of abstracts. - Bratislava, Slovakia: Slovak Clay Group, 2019, p. 13-14. ISBN 978-80-972367-3-1. (Workshop of Slovak Clay Group).

SCHOLTZOVÁ, Eva. Computational study of Cs-hectorite. In 6th Workshop of Slovak Clay Group: Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia: book of abstracts. - Bratislava, Slovakia: Slovak Clay Group, 2019, p. 17-18. ISBN 978-80-972367-3-1. (Workshop of Slovak Clay Group).

ŠKORŇA, Peter - SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - TUNEGA, Daniel. Structural and spectroscopic characterization of beidellite intercalated with choline and acetylcholine. In 6th Workshop of Slovak Clay Group: Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia: book of abstracts. - Bratislava, Slovakia: Slovak Clay Group, 2019, p. 21-22. ISBN 978-80-972367-3-1.

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

Zodpovedný riešiteľ: František Šimko
Trvanie projektu: 1.1.2018 / 31.12.2021
Evidenčné číslo projektu: 2/0060/18
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: SAV: 9364 €

Dosiahnuté výsledky:

Uskutočnila sa komplexná analýza správania sa pseudobinárnych systémov $\text{MF}-\text{Al}_2\text{O}_3$, v závislosti od zloženia a teploty. Vo všetkých systémoch bola pozorovaná prítomnosť štyroch už známych fáz, a to prítomnosť MF , M_3AlF_6 , MAlO_2 a $\text{M}_2\text{Al}_2\text{O}_3\text{F}_2$ ($\text{M}=\text{K}, \text{Rb}, \text{Cs}$). Okrem toho boli identifikované nové fázy, a to $\text{M}_2\text{Al}_2\text{O}_3\text{F}_2$ ($\text{M}=\text{Rb}, \text{Cs}$), pričom sa stanovila aj ich štruktúra. Pozoruhodnou charakteristikou kryštálovej štruktúry oboch pripravených komplexov je prítomnosť vrstiev, zložených z jednotlivých (AlO_3F) tetredrov, zdieľajúcich navzájom spoločné rohy, v ktorých sú umiestnené atómy kyslíka, zatiaľ čo atómy fluóru oddeľujú jednotlivé vrstvy. Počet a množstvo neekvivaletných kryštalografických polôh jednotlivých atómov, prítomných v uvedenej štruktúre sa určil pomocou ^{19}F , ^{27}Al , ^{87}Rb a ^{133}Cs MAS NMR spektier v tuhom stave. Získaná fáza, $\text{Rb}_2\text{Al}_2\text{O}_3\text{F}_2$, vykazovala aj určitú iónovú vodivosť pri izbovej teplote hodnoty $1,74 \times 10^{-5} \text{ S cm}^{-1}$. Pomocou termickej analýzy sa zistilo, že analyzované, pseudobinárne systémy $\text{MF}-\text{Al}_2\text{O}_3$ sa chovajú ako stabilné diagonálne časti komplexných kvartérnych systémov $\text{MF}-\text{AlF}_3-\text{Al}_2\text{O}_3-\text{M}_2\text{O}$ ($\text{M}=\text{K}, \text{Rb}, \text{Cs}$), so základným iónovými zložkami (M^+ , Al^{3+} , O^{2-} a F^-), zodpovednými za tvorbu pozorovaných komplexných zlúčenín. Novo objavená fáza, $\text{Rb}_2\text{Al}_2\text{O}_3\text{F}_2$, bola prítomná v celom koncentračnom rozsahu skúmaného systému. Zistilo sa, že so zmenou teploty sa čiastočne rozkladá na oxohlinitan rubídny ($\text{Rb}_2\text{Al}_2\text{O}_3\text{F}_2$), ktorý má podobné štruktúrne usporiadanie ako $\text{Rb}_2\text{Al}_2\text{O}_3\text{F}_2$, a na príslušnú fluoridovú fázu (Rb_3AlF_6 , RbF). Nestabilita oxofluorohlinitanu rubídneho pravdepodobne súvisí s uvedenou štruktúrnou podobnosťou $\text{Rb}_2\text{Al}_2\text{O}_3\text{F}_2$ a $\text{Rb}_2\text{Al}_2\text{O}_3\text{F}_2$, ktorá bola zistená a potvrdená NMR analýzou v tuhej fáze. Následne sa stanovila elektrická vodivosť roztavených fluoridových komplexných zlúčenín, K_3AlF_6 , Rb_3AlF_6 , Cs_3AlF_6 a CsF . Zistilo sa, že elektrická vodivosť roztaveného K_3AlF_6 je $2,64 \text{ S cm}^{-1}$ pri 1000°C . Zistilo sa, že elektrická vodivosť roztaveného Rb_3AlF_6 je $2,06 \text{ S cm}^{-1}$ pri 1000°C . Vodivosť roztaveného Cs_3AlF_6 pri rovnakej teplote je $1,36 \text{ S cm}^{-1}$, pretože sa zistilo, že vodivosť CsF pri 1000°C je $2,57 \text{ S cm}^{-1}$. Zistilo sa, že hodnoty elektrickej vodivosti neustále klesajú v smere od $\text{K}_3\text{AlF}_6 > \text{Rb}_3\text{AlF}_6 > \text{Cs}_3\text{AlF}_6$. Tento pokles vodivosti je pravdepodobne spôsobený nárastom veľkosti a hmotnosti katiónov.

Publikácie a príspevky:

ŠIMKO, František - RAKHMATULLIN, Aydar - VÉRON, Emmanuel - ALLIX, Mathieu - FLORIAN, Pierre - KORENKO, Michal - NETRIOVÁ, Zuzana - BESSADA, Catherine. Oxo- and (oxo)(fluoro)-aluminates: Synthesis, stability and structure correlation = Oxo- a (oxo)(fluoro)-hlinitany: Syntézy, stabilita a vzájomná štruktúrna korelácia. In Interakce tavenin s progresivními anorganickými materiály, 10. odborný seminář, 14. - 15. října 2019, Hradec nad Moravicí, Česká republika. - Česká republika: VŠB TU Ostrava, 2019, p. 11-13.

ŠIMKO, František - RAKHMATULLIN, Aydar - VERON, Emmanuel - ALLIX, Mathieu - FLORIAN, Pierre - NETRIOVÁ, Zuzana - KORENKO, Michal - KAVEČANSKÝ, Viktor - BESSADA, Catherine. Oxo- and (oxo)(fluoro)-aluminates: Synthesis, stability and structure correlation. In MS11. 11th international symposium on molten salts - chemistry and technology, 19-23 Mai 2019, Orleans, France: program and abstracts. - France, 2019, p. 26.

ŠIMKO, František - RAKHMATULLIN, Aydar - VÉRON, Emmanuel - ALLIX, Mathieu - FLORIAN, Pierre - BUČKO, Tomáš - NETRIOVÁ, Zuzana - KORENKO, Michal - BESSADA, Catherine. Fluoro-, oxo- and oxofluoro-aluminates: Synthesis, and their stability. In ChemZi: Zborník abstraktov: 71. Zjazd chemikov, 9-13 september 2019, Vysoké Tatry, Horný Smokovec, Slovensko. Bratislava: Slovenská chemická spoločnosť, 2019, 2019, roč. 15, č. 1, s. 174. ISSN 1336-7242.

Programy: APVV

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

Zodpovedný riešiteľ:	Miroslav Boča
Trvanie projektu:	1.7.2016 / 30.6.2020
Evidenčné číslo projektu:	APVV-15-0479
Organizácia je koordinátorom projektu:	áno
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	0
Čerpané financie:	APVV: 60000 €

Dosiahnuté výsledky:

Bola uskutočnená fyzikálno-chemická analýza viacerých roztavených fluoridových systémov s obsahom MgO . Pre tieto sústavy bola meraná rozpustnosť, hustota, elektrická vodivosť a viskozita. Bolo zistené, že rozpustnosť oxidu horečnatého je nízka vo všetkých študovaných systémoch a je pod $0,5 \text{ mol.}\%$ MgO . Hustota na báze horečnatých roztavených sústav bola meraná pre dva systémy: $(\text{CaF}_2\text{-MgF}_2)\text{eut-MgO}$ a $(\text{CaF}_2\text{-MgF}_2\text{-LiF})\text{eut-MgO}$. Výsledky ukázali, že experimentálne hodnoty hustôt v oboch prípadoch lineárne klesajú s teplotou. Vplyv prídavku MgO do roztavených systémov $(\text{CaF}_2\text{-MgF}_2)\text{eut}$ a $(\text{CaF}_2\text{-MgF}_2\text{-LiF})\text{eut}$ je však rozdielny. V prvom prípade bol pozorovaný malý pozitívny vplyv; hodnoty

hustôt sa menili do 1%, kým v prípade ($\text{MgF}_2 - \text{CaF}_2 - \text{LiF}$) eutektickej zmesi, prídavok MgO mal výrazný negatívny vplyv (7-9%). Ešte výraznejší rozdiel vplyvu prídavku MgO do týchto dvoch roztavených zmesí je badateľný v prípade koncentračnej závislosti molárneho objemu. V sústavách bez fluoridu lítneho molárny objem klesá s prídavkom MgO , v sústavách s fluoridom lítnym bol pozorovaný opačný trend, molárny objem narastá s prídavkom MgO . Vysvetlením pre takéto správanie môže byť rozdielne vnútorné usporiadanie týchto tavenín, kde v sústavách bez LiF oxid horečnatý vytvára komplexné častice približne rovnakej veľkosti, v sústavách s fluoridom lítnym MgO tvorí komplexné častice rôznej veľkosti. Výsledky z merania elektrickej vodivosti sústavy $\text{MgF}_2 - \text{CaF}_2 - \text{MgO}$ ukázali, že nárast pomeru $\text{MgF}_2/\text{CaF}_2$ má negatívny vplyv na elektrickú vodivosť taveniny. Pozitívny vplyv na túto vlastnosť bol pozorovaný v prípade nárastu obsahu MgF_2 . Ďalšou študovanou fyzikálno-chemickou vlastnosťou bola viskozita meraná pre eutektické zloženie ($\text{MgF}_2 - \text{CaF}_2$)eut. Výsledky ukázali, že viskozita tohto binárneho systému je relatívne vysoká.

Publikácie a príspevky:

KORENKO, Michal - ŠIMKO, František - MLYNÁRIKOVÁ, Jarmila - LARSON, Carol - MIKŠÍKOVÁ, Eva - PRIŠČÁK, Jozef - AMBROVÁ, Marta - PALUMBO, Robert. Physico-chemical properties of ($\text{MgF}_2 - \text{CaF}_2 - (\text{LiF})$)eut- MgO system as a molten electrolyte for Mg electrowinning. In Journal of Molecular Liquids, 2019, vol. 275, p. 535-543. (4.561 - IF2018). (2019 - Current Contents, WOS, SCOPUS). ISSN 0167-7322. Typ: ADCA

KORENKO, Michal - ŠIMKO, František - MLYNÁRIKOVÁ, Jarmila - LARSON, Carol - MIKŠÍKOVÁ, Eva - PRIŠČÁK, Jozef - PALUMBO, Robert - AMBROVÁ, Marta. Physico-chemical properties of ($\text{MgF}_2 - \text{CaF}_2 - (\text{LiF})$)eut- MgO system as a molten electrolyte for solar thermal Mg electrowinning. In MS11. 11th international symposium on molten salts - chemistry and technology, 19-23 Mai 2019, Orleans, France: program and abstracts. - France, 2019, p. 58. Typ: AFG

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

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

Dosiahnuté výsledky:

V rámci nových experimentov sa podarilo pripraviť niekoľko typov modifikovaných polymérov s aktívnym povrchom, čo sa dosiahlo modifikáciou s vrstevnatými silikátmi, ktorých častice boli funkcionalizované fotoaktívnymi farbivami. Dokázalo sa, že použitie fluorescenčných polymérov môže pomôcť pri zužitkovaní širokého spektra viditeľného svetla pre efektívnejšiu fotosenzibilizáciu (1). Doposiaľ nebolo jasné, prečo metylénová modrá, napriek zníženej fotoaktivity vykazuje lepšie antimikrobiálne vlastnosti v hybridných systémoch so silikátmi. Dokázalo sa, že častice silikátov môžu aktívne ovplyvňovať chemické vlastnosti adsorbovaných molekúl farbív (2). Príkladom je stabilizácia metylénovej modrej, ktorej redukcia neprebíhala v adsorbovanom stave. Práve tento jav môže zohrávať kľúčovú úlohu pri antimikrobiálnych vlastnostiach hybridných systémov fotosenzibilizačných farbív a vrstevnatých silikátov (2). V tejto súvislosti sme sa zaoberali aj vplyvom adsorpcie buniek baktérií na častice silikátov, a nové výsledky boli súčasťou publikácie (3).

1. LACKOVIČOVÁ, Monika - BARANYAIOVÁ, Tímea - BUJDÁK, Juraj**. The chemical stabilization of methylene blue in colloidal dispersions of smectites. In Applied Clay Science, 2019, vol. 181, no., p. 105222-1-105222-8. (2018: 3.890 - IF, Q1 - JCR, 0.990 - SJR, Q1 - SJR, karentované - CCC).

2. KUREKOVÁ, Valéria - BELUŠÁKOVÁ, Silvia - BOHÁČ, Peter - BUJDÁK, Juraj**. Resonance energy transfer in the systems of smectite modified with a fluorescent cationic polymer and a photosensitizer. In Applied Clay Science, 2019, vol. 183, no., p. 105326-1-105326-9. (2018: 3.890 - IF, Q1 - JCR, 0.990 - SJR, Q1 - SJR, karentované - CCC).

3. GAÁLOVÁ, Barbora - VYLETELOVÁ, Ivana - POKORNÁ, Katarína - KIKHNEY, Judith - MONET, Annette - BUJDÁK, Juraj - BUJDÁKOVÁ, Helena**. Decreased vitality and viability of Escherichia coli isolated by adherence to saponite particles. In Applied Clay Science, 2019, vol. 183, p. 105316-1-105316-9. (2018: 3.890 - IF, Q1 - JCR, 0.990 - SJR, Q1 - SJR, karentované - CCC).

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

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

Dosiahnuté výsledky:

Na základe výsledkov nadobudnutých počas riešenia projektu v minulých rokoch, bola hlavná aktivita venovaná optimalizácii procesu prípravy materiálov na báze TiB₂ s prídavkom rôzneho obsahu grafénových nanoplátčiek (1, 2, 5, a 10 hm.%). Proces zhutnenia týchto materiálov, t.j. mechanizmus a kinetika spekania, bol porovnaný s procesom spekania kompozitných TiB₂-SiC materiálov s rovnakým množstvom prísad grafénových nanoplátčiek, ktoré boli v predchádzajúcom období riešenia projektu pripravené a študované. Za veľmi pozitívny výsledok možno považovať skutočnosť, že po optimalizácii procesu prípravy sa podarilo získať hutné vzorky aj bez nutnosti použitia prísady SiC. V nasledujúcom období budú tieto vzorky podrobené fázovej a mikroštruktúrnej analýze, a ich mechanické vlastnosti budú porovnané s materiálmi TiB₂-SiC s prídavkom grafénových nanoplátčiek.

Výstupy:

1. KOVALČÍKOVÁ, Alexandra - TATARKO, Peter - SEDLÁK, Richard - MEDVEĎ, Dávid - HÚLAN, Michal - MÚDRA, Erika - IVOR, Michal - DUSZA, Ján. Mechanical and tribological properties of TiB₂-SiC-GPLs ceramic composites. In CICC-11: The Eleventh International Conference on High-Performance Ceramics, May 25-29, 2019, Kunming, China: abstract book. - China: The Chinese Ceramic Society, 2019, p. 86. Typ: AFG
2. KOVALČÍKOVÁ, Alexandra - TATARKO, Peter - MEDVEĎ, Dávid - SEDLÁK, Richard - CHLUP, Zdeněk - MÚDRA, Erika - DUSZA, Ján. Effect of graphene platelets on mechanical and tribological properties of TiB₂-SiC-GPLs ceramic composites. In Fractography of advanced ceramics FAC 2019: The International conference. Book of abstracts. Smolenice, 8.-11.9.2019, ISBN 978-80-89782-12-3. Typ: AFH

16.) Kompozitné vrstvy pre vysokoteplotnú protikoróznú ochranu kovov (*Advanced composite coatings for high temperature corrosion protection of metals*)

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

Dosiahnuté výsledky:

1. Vývoj optimálnej metodiky čistenia oceľových substrátov na zabezpečenie adhézie povlakov k oceľovému substrátu.
2. Vývoj kompozitnej vrstvy na báze PDC so sklenými a keramickými pasívnymi plnivami s vysokou adhéziou k oceľovému substrátu a vysokou odolnosťou voči oxidácii pri teplotách do 1000 °C.
3. Verifikácia koróznej odolnosti povlakovaných ocelí pomocou dlhodobých oxidačných testov a určenie parametrov zodpovedných za zvýšenie odolnosti antikorózných vrstiev.

Publikácie:

1. I. Petříková, M. Parchovianský, P. Švančárek, M. Lenz leite, G. Motz, D. Galusek, Passive filler loaded polysilazane-derived glass/ceramic coating system applied to AISI 441 stainless steel, part 1: Processing and characterization. Int. J. Appl. Ceram. Technol., 1-12, (2019), DOI: 10.1111/ijac.13417
2. Milan Parchovianský, Ivana Petříková, Peter Švančárek, Mateus Lenz Leite, Günter Motz, Dušan Galusek, Passive

Filler loaded PDC coating system applied to AISI 441 stainless steel, Part 2: Corrosion behaviour, Int. J. Appl. Ceram. Technol, submitted

17.) Nové sklenené a sklokeramické fosfory na báze hlinitanov vzácnych zemín pre aplikácie v pevnolátkových energiách 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: 12960 €

Dosiahnuté výsledky:

1. Príprava luminoforov vo forme mikroguľôčok v sústave YAG-Al₂O₃ dopovaných PL aktívnymi iónmi Ce³⁺ a Eu²⁺ - efekt koncentrácie na PL vlastnosti.
2. Štúdium kinetiky kryštalizácie skiel v sústave YAG-Al₂O₃.
3. Optimalizácia prípravy kompakto luminoforov zo sklených mikroguľôčok žiarovým lisovaním – optimalizácia časovo-teplotného režimu, štúdium vplyvu procesných podmienok (teploty spekania) na optické a luminiscenčné vlastnosti pripravených kompakto.
4. Štúdium optických a fotoluminiscenčných vlastností luminoforu emitujúceho červené svetlo v transparentnej keramike Al₂O₃:Cr³⁺ - efekt koncentrácie dopantu.

Publikácie

1. Anna Prnová, Jana Valúchová, Milan Parchovianský, Wolfgang Wisniewski, Peter Švančárek, Robert Klement, Ľubomír Hric, Els Bruneel, Dušan Galusek: Y₃Al₅O₁₂-Al₂O₃ composites with fine-grained microstructure by hot pressing of Al₂O₃-Y₂O₃ glass microspheres, J. Eur. Ceram. Soc. 40(3) (2020), 852-860.
2. Katarína Drdliková, Robert Klement, Daniel Drdlik, Dušan Galusek, Karel Maca: Processing and properties of luminescent Cr³⁺ doped transparent alumina ceramics, J. Eur. Ceram. Soc. In press (<https://doi.org/10.1016/j.jeurceramsoc.2019.11.010>).

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

Zodpovedný riešiteľ: Miroslav Hnatko
Trvanie projektu: 1.7.2016 / 30.6.2020
Evidenčné číslo projektu: APVV-15-0540
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: APVV: 44137 €

Dosiahnuté výsledky:

V priebehu realizácie projektu boli získané poznatky a dosiahnuté výsledky v oblastiach vyselektovaných na základe potenciálneho využitia druhotných surovín v predchádzajúcich rokoch.

(i) Ľahké kamenivo, t.j. kamenivo s hustotou nižšou ako 2 g.cm⁻³, bolo pripravené z „odpadov“ technologických prúdov oceliarskeho a ferozliatinového priemyslu. Optimalizáciou syntézy pri 1250 °C v ochrannnej atmosfére Ar boli pripravené agregáty s majoritným podielom SiC a „skelnej“ (sklokeramickej) fázy, ktorej prítomnosť zvýšila zhutnenie agregátov ako aj dosiahnutie vhodnej pevnosti. Hustota pripravených agregátov dosahovala hodnotu 1.253 g.cm⁻³ a pevnosť v tlaku 5.13 MPa. Optimalizáciou tohto prístupu bolo možné kombináciou odpadov ako druhotných surovín pripraviť materiál s pridanou hodnotou využiteľný ako ľahké kamenivo pre potenciálnu priemyselnú aplikáciu v špeciálnych betónoch.

(ii) V oblasti keramicko-cementových kompozitov bol optimalizovaný prístup kombinácie druhotných surovín (odpadov) na báze popolčekov v kombinácii s bežne dostupným portlandským cementom (PC). Kombináciou druhotných surovín s vyšším obsahom SiO₂, PC a vhodného aktivátora bolo možné dosiahnuť zvýšenú puzolánovú aktivitu takejto zmesi a teda tvorbu hydratovaných kremičitanov, ktoré následným tepelným spracovávaním pri reálnych nízkych teplotách (do 1000°C) pôsobia ako spekacia prísada a v konečnom dôsledku spevňujú štruktúru vzniknutého kompozitu (zvýšenie pevnosti).

Publikácie:

BYSTRICKÝ, Roman - HNATKO, Miroslav - SEDLÁČEK, Jaroslav. Preparation of lightweight aggregates from industrial waste. In Preparation of ceramic materials: Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. Košice Technical University, 2019, p. 33-37. ISBN 978-80-553-3314-4. AFD

HNATKO, Miroslav - HIČÁK, Michal - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Surface modification of dense silicon nitride. In Preparation of ceramic materials: Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. Košice Technical University, 2019, p. 103-109. ISBN 978-80-553-3314-4. AFD

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

Zodpovedný riešiteľ:	Luboš Jankovič
Trvanie projektu:	1.7.2016 / 30.6.2020
Evidenčné číslo projektu:	APVV-15-0741
Organizácia je koordinátorom projektu:	áno
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	1 - Slovensko: 1
Čerpané financie:	APVV: 40000 €

Dosiahnuté výsledky:

Riešenie projektu postupuje podľa schváleného harmonogramu. V roku 2019 sa riešili úlohy, ktoré patria čiastočne do tretej (05/2018 – 07/2019) a štvrtej (01/2019 – 06/2020) etapy. Pripravila sa kompaktná séria organoílov na báze syntetických (komerčne nedostupných) trimetylalkylfosfóniových kationov s rôznou dĺžkou alkylového reťazca (Me3P-C2 až Me3P-C20). Paralelne k tejto sade sa pripravila séria organo-montmorillonitov (O-Mt) z tributylalkyl-fosfóniových (Bu3P-CX) a tributylalkylamóniových (Bu3N-CX) kationov (X = 4, 8, 12 a 16) a uskutočnila sa ich základná charakterizácia a vyhodnotenie vlastností vzhľadom na typ centrálného atómu a dĺžku alkylového reťazca. Na syntetických smektitoch interkalovaných tetraoktylamóniovým (Oct4N) a tetraoktylfosfóniovým (Oct4P) kationom, sytených v rôznom stupni vzhľadom na kationovýmennú kapacitu (KVK) pôvodného smektitu, sa sledoval vplyv surfaktantu a typu smektitu na expanziu medzivrstvového priestoru, termickú a mechanickú stabilitu, ako aj na luminiscenčné aj hydratačné vlastnosti pripravených organoílov. Boli ukončené experimenty a interpretácia výsledkov na sérii organoílov modifikovaných C1-NH₃ (metyl-) až C19-NH₃ (nonadecyl-) kationmi [1], ktoré sa porovnávajú s vlastnosťami organoílov s interkalovanými syntetickými fosfóniovými Me3P-C2 - Me3P-C20 kationmi, ktoré majú podobnú dĺžku alkylového reťazca. V rámci riešenia úloh zameraných na interakcie organoílov s fluorescenčnými farbivami sa pripravili a charakterizovali hybridné materiály zložené zo saponitu, fotosenzibilizačného farbiva floxínu B a polysacharidu modifikovaného kladnými amóniovými skupinami a označeného fluoresceínovým luminofórom. Takéto materiály majú potenciálne využitie ako antimikrobiálne fotosenzibilizačné materiály [2]. Sledoval sa aj vplyv častíc smektitu na redox reakciu medzi metylénovou modrou a kyselinou askorbovou vo vodných roztokoch a koloidných sústavách [3]. Aplikáciou *Ab initio* molekulovej dynamiky na DFT úrovni sa skompletizovala štúdia opisu väzbových a štruktúrnych pomerov montmorillonitu interkalovanom dvomi typmi organických kationov, tetrabutylfosfóniovým a tetrabutylamóniovým [4]. Uskutočnila sa kompletná charakterizácia in vitro toxicity pripravených alkylfosfóniových solí. Dôvodom bolo ich použitie v biodegradovateľných polyméroch, čo otvára možnosť využitia pre biomedicínske účely. Interkaláciou štyroch komerčne dostupných surfaktantov alkylfosfóniových solí sa pripravili O-Mt, ktoré sa následne použili na prípravu polymérno-flových kompozitov. Vzorky O-Mt v rozličnej koncentrácii sa budú testovať ako plnivá vo vybraných polymérnych matriciach. Vlastnosti nanokompozitov sa porovnávajú s analogickými materiálmi na báze amóniových kationov.

Publikácie:

[1] SLANÝ, Michal - JANKOVIČ, Luboš - MADEJOVÁ, Jana. Structural characterization of organo-montmorillonites prepared from a series of primary alkylamines salts: Mid-IR and near-IR study. In Applied Clay Science, 2019, vol. 176, p. 11-20. (3.890 - IF2018).

- [2] BIZOVSKÁ KUREKOVÁ, Valéria - BELUŠÁKOVÁ, Silvia - BOHÁČ, Peter - BUJDÁK, Juraj. Resonance energy transfer in the systems of smectite modified with a fluorescent cationic polymer and a photosensitizer. In *Applied Clay Science*, 2019, vol. 183, no., p. 105326-1-105326-9. (3.890 - IF2018).
- [3] LACKOVIČOVÁ, Monika - BARANYAIOVÁ, Tímea - BUJDÁK, Juraj. The chemical stabilization of methylene blue in colloidal dispersions of smectites. In *Applied Clay Science*, 2019, vol. 181, no., p. 105222-1-105222-8. (3.890 - IF2018).
- [4] SCHOLTZOVÁ, Eva - TUNEGA, Daniel. Density functional theory study of the stability of the tetrabutylphosphonium and tetrabutylammonium montmorillonites. In *Clay Minerals*, 2019, vol. 54, no. 1, p. 41-48. (1.787 - IF2018).

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

Zodpovedný riešiteľ:	Zoltán Lenčes
Trvanie projektu:	1.7.2015 / 30.6.2019
Evidenčné číslo projektu:	APVV-14-0385
Organizácia je koordinátorom projektu:	áno
Koordinátor:	Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií:	2 - Slovensko: 2
Čerpané financie:	APVV: 17617 €

Dosiahnuté výsledky:

Podrobnejšie boli študované luminiscenčných vlastností spinelu (MgAl_2O_4) dopovaného Cr^{3+} . Cieľom bolo overiť možnosť náhrady drahých dopantov z radu lantanoidov lacnejšími prechodnými prvkami. Luminofor $\text{MgAl}_2\text{O}_4:\text{Cr}^{3+}$ vykazoval slabú emisiu s maximom pri 370 nm (fialové svetlo) po excitácii $\lambda_{\text{ex}} = 250$ nm. Po excitácii zeleným svetlom ($\lambda_{\text{ex}} = 500 - 550$ nm) bola nameraná silná emisia v tmavo-červenej oblasti viditeľného svetla s maximom pri 690 - 710 nm.

Študoval sa aj vplyv množstva Eu v koncentračnom rozsahu 0,5 mol% až 3 mol% na luminiscenčné vlastnosti spinelu MgAlON (tuhý roztok MgAl_2O_4 a AlN). Emisné spektrá vzoriek po excitácii 350 nm žiarením mali maximum emisie je pri 472 nm (modré svetlo). Z výsledkov vyplýva, že najvyššia intenzita emitovaného žiarenia bola dosiahnutá v prípade MgAlON vzorky dopovanej 0,5 mol% Eu, potom pri zvyšujúcom sa obsahu Eu dochádzalo ku koncentračnému zhášaniu. V porovnaní so vzorkou $\text{MgAl}_2\text{O}_4:\text{Eu}$ ($\lambda_{\text{em,max}} = 460$ nm) došlo k červenému posuvu maxima v dôsledku prítomnosti dusíka v štruktúre a zvýšeniu kovalentnosti väzieb v blízkom okolí dopantu.

Bola vykonaná aj sada experimentov s cieľom pripraviť luminofor na báze O'-sialonu (všeobecný vzorec $\text{Si}_{2-x}\text{Al}_x\text{O}_{1+x}\text{N}_{2-x}$). Zo zmesi Si_3N_4 a polymérneho prekurzoru SiAlOC sa podarilo pripraviť luminofor O'-sialon dopovaný cérom (Ce^{3+}) žiarovým lisovaním pri 1720 °C po dobu 15 min, mechanickom tlaku 30 MPa a následným žihaním pri 1620 °C po dobu 3 h v atmosfére dusíka (2 MPa). Po excitácii luminoforu UV žiarením bola pozorovaná emisia v zelenej oblasti svetla s maximom pri 534 nm.

V rámci riešenia projektu vznikla aj spolupráca s Functional Ceramics Laboratory, Department of Materials Science and Engineering, University of Seoul, (prof. Young-Wook Kim) na vývoji keramických substrátov pre LED aplikácie.

Publikácie:

Young-Wook Kim, Shynar Kultayeva, Jaroslav Sedláček, Ondrej Hanzel, Peter Tatarko, Zoltán Lenčes, Pavol Šajgalík: Thermal and electrical properties of additive-free rapidly hot-pressed SiC ceramics. *J. Eur. Ceram. Soc.*, 40 (2020) 234-240.

Y. Duan, J. Zhang, X. Li, H. Bai, P. Šajgalík, D. Jiang, High thermal conductivity silicon nitride ceramics prepared by pressureless sintering with ternary sintering additives. *Int. J. Appl. Ceram. Technol.*, (2019) 1-8. <https://doi.org/10.1111/ijac.13220>

O. Hanzel, M.A. Singh, D. Marla, R. Sedlák, P. Šajgalík, Wire electrical discharge machinable SiC with GNPs and GO as the electrically conductive filler. *J. Eur. Ceram. Soc.*, 39 (2019) 2626-2633. <https://doi.org/10.1016/j.jeurceramsoc.2019.03.012>

O. Hanzel, Z. Lenčes, Y.-W. Kim, J. Fedor, P. Šajgalík, High electrically and thermally conductive silicon carbide – graphene composites with yttria and scandia additives. *J. Eur. Ceram. Soc.*, (2019) under review. Manuscript Ref. No.:

JECS-D-19-01506

LENČEŠ, Zoltán - RADWAN, Mohamed - ŠAJGALÍK, Pavol. Preparation of transparent MgAl_2O_4 ceramics for LED applications. In ICACC 2019. 43rd International Conference & Exposition on Advanced Ceramics and Composites, January 27 - February 1, 2019, Daytona Beach, Florida, USA: abstract book. USA: The American Ceramic Society, 2019, p. 36. (ICACC 2019. International Conference & Exposition on Advanced Ceramics and Composites).

Z. Lenčėš, M. Radwan, A. Czimerov , P. Šajgal k, Preparation of transparent/translucent spinel-based phosphors. Abstract Book of the XVIth Conference and Exhibition of the European Ceramic Society, 16-20 June 2019, Torino, Societa Ceramica Italiana, p. 507.

LENČEŠ, Zolt n - CZ MEROV , Adriana - PETRISKOV , Patr cia - KLEMENT, R bert - HULMAN, Martin. Influence of lanthanide oxides and fluorides on the photoluminescence of LaSi_3N_5 . In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019: book of abstracts. - Bratislava, Slovakia: Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 79. ISBN 978-80-971648-7-4.

PETRISKOV , Patr cia - RADWAN, Mohamed - MONFORT, O. - PLESCH, Gust v - LENČEŠ, Zolt n. Photocatalytic TiO_2 nanotubes arrays formation on polymeric and ceramic substrates. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019: book of abstracts. - Bratislava, Slovakia: Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 81. ISBN 978-80-971648-7-4.

21.) V voj nov ch teoretick ch n strojov pre predikciu a interpret ciu EPR a NMR parametrov (Developing new theoretical tools for prediction and interpretation of EPR and NMR parameters)

Zodpovedn  rie itel': Vladim r Malkin
Trvanie projektu: 1.7.2016 / 30.6.2020
Eviden n    slo projektu: APVV-15-0726
Organiz cia je koordin torom projektu:  no
Koordin tor:  stav anorganickej ch mie SAV
Po et spolurie itel'sk ch in tituc  : 1 - Slovensko: 1
 erpan  financie: APVV: 40200  

Dosiahnut  v sledky:

KOMOROVSK , Stanislav – CHERRY, Peter – REPISK , Michal. Four-component relativistic time-dependent density-functional theory using a stable noncollinear DFT ansatz applicable to both closed- and open-shell systems. In Journal of Chemical Physics, 2019, vol. 151, no. 18, p. 184111-1-184111-14. (2.997 – IF2018). ISSN 0021-9606. Typ: ADCA

22.) Povrchy polym rov modifikovan  vrstevnat mi nano asticami a fotoakt vnymi farbivami (Polymer surfaces modified with layered nanoparticles and photoactive dyes)

Zodpovedn  rie itel': Helena P lkov 
Trvanie projektu: 1.7.2019 / 30.6.2023
Eviden n    slo projektu: APVV-18-0075
Organiz cia je koordin torom projektu: nie
Koordin tor:  stav anorganickej ch mie SAV
Po et spolurie itel'sk ch in tituc  : 1 - Slovensko: 1
 erpan  financie: APVV: 5600  

Dosiahnut  v sledky:

V prvom polroku rie enia projektu prebehlo zaobstaranie farb v a surfaktantov. Za ali sa pilotn  experimenty, v ktor ch sa realizovala pr prava a charakteriz cia niektor ch typov hybridn ch materi lov na b ze organick ch zl u en   a vrstevnat ch hydrosilik tov. Otestovali sa niektor  komer ne dostupn  polym ry a schopnosť vrstevnat ch  ast   vytvoriť kompaktn  film s polym rom a niektor mi z kladn mi farbivami.

23.) Vlastnosti nov ch progres vn ch kon truk n ch materi lov v agres vnom prostred  roztaven ch sol  (The behaviour of new progressive construction materials in aggressive environment of molten salts)

Zodpovedn  rie itel': Franti ek Šimko

Trvanie projektu: 1.7.2016 / 30.6.2020
Evidenčné číslo projektu: APVV-15-0738
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 1 - Slovensko: 1
Čerpané financie: APVV: 35000 €

Dosiahnuté výsledky:

Projekt je zameraný na možné zachytenie metastabilných fáz z roztavených fluorových tavenín. Metóda extrémne rýchleho chladenia (melt spinning; typicky používaná pre tvorbu kovových skiel) bola aplikovaná na zachytenie a prípravu metastabilných fáz z roztavených fluoridových tavenín; konkrétne zo systému zloženia $(\text{LiF}-\text{CaF}_2)_{\text{eut}}-x\text{LaF}_3$ ($x = 0, 5, 10, 20, \text{ a } 30 \text{ mol}\%$). Touto metódou boli pripravené dva typy podchladených fragmentov – tvaru šupiniek a sférického tvaru. Fázová analýza doplnená o SEM-EDX a S/TEM analýzu potvrdila existenciu metastabilnej fázy obsahujúcej prvky Ca, La a F. Táto fáza súvisí so známou fcc $\text{Ca}_{0.65}\text{La}_{0.35}\text{F}_{2.35}$ fázou. Mriežkové parametre metastabilnej fázy sa menili so zložením ochladzovaného systému. Bolo zistené, že po teplotnej relaxácii sa metastabilná fáza rozpadá na CaF_2 a LaF_3 , čo je v súlade s rovnovážnym fázovým diagramom študovaného systému. Pozorovanie tvorby dodatočnej/zdanlivej fázy v nerovnovážnom stave demonštruje využitie extrémne rýchleho chladenia na dosiahnutie a štúdium teplotne nerovnovážnych stavov tuhých látok, čo odráža akýsi zamrznutý stav kvapaliny.

Publikácie a príspevky:

BOČA, Miroslav - ŠIMURDA, Michal - ŠVEC, Peter - ŠVEC, Peter Jr. - JANIČKOVIČ, Dušan - CZÍMEROVÁ, Adriana - KUBÍKOVÁ, Blanka - MLYNÁRIKOVÁ, Jarmila. Unexpected phase transformations in ternary fluoride systems. In 19th European Symposium on Fluorine Chemistry: Book of Abstracts. - Warszawa, Poland: Oficyna Wydawnicza-Poligraficzna ADAM, 2019, p. 134.

BOČA, Miroslav - ŠIMURDA, Michal - ŠVEC, Peter - ŠVEC, Peter Jr. - JANIČKOVIČ, Dušan - CZÍMEROVÁ, Adriana - KUBÍKOVÁ, Blanka - MLYNÁRIKOVÁ, Jarmila. Unusual phase transformations in ternary fluoride systems. In MS11. 11th international symposium on molten salts - chemistry and technology, 19-23 Mai 2019, Orleans, France: program and abstracts. - France, 2019, p. 87.

BOČA, Miroslav - ŠIMURDA, Michal - ŠVEC, Peter - ŠVEC, Peter Jr. - JANIČKOVIČ, Dušan - CZÍMEROVÁ, Adriana - KUBÍKOVÁ, Blanka - NETRIOVÁ, Zuzana - MLYNÁRIKOVÁ, Jarmila. Unusual phase transformations in ternary fluoride systems. In ChemZi: Zborník abstraktov: 71. Zjazd chemikov, 9-13 september 2019, Vysoké Tatry, Horný Smokovec, Slovensko. Bratislava: Slovenská chemická spoločnosť, 2019, 2019, roč. 15, č. 1, s. 82. ISSN 1336-7242. Typ: AFH

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

Zodpovedný riešiteľ: Peter Tatarko
Trvanie projektu: 1.8.2018 / 30.6.2022
Evidenčné číslo projektu: APVV-17-0328
Organizácia je koordinátorom projektu: áno
Koordinátor: Ústav anorganickej chémie SAV
Počet spoluriešiteľských inštitúcií: 0
Čerpané financie: APVV: 45863 €

Dosiahnuté výsledky:

Riešenie projektu pokračovalo optimalizáciou procesu spekania materiálov na báze diboridovej keramiky $\text{ZrB}_2\text{-SiC}$ s prídavkom rôzneho obsahu rôznych oxidov prvkov vzácnych zemín. Na základe výsledkov spekania (kinetika, hustota vzoriek) bol ako najoptimálnejší spôsob prípravy určený spekanie pri podmienkach $2000^\circ\text{C}/70\text{MPa}/7\text{min}/\text{Ar}$ pre materiály s prídavkom 2 a 5 hmot.% prísad. Nakoľko oxidy vzácnych zemín podporovali spekanie, materiály s obsahom 10 hmot.% boli spekané pri nižšej teplote, t.j. pri podmienkach: $1950^\circ\text{C}/70\text{MPa}/7\text{min}/\text{Ar}$. Všetky materiály dosiahli relatívnu hustotu viac ako 98% teoretickej hustoty. Boli študované mechanické vlastnosti týchto materiálov pri izbovej teplote, akými sú pevnosť, Youngov modul pružnosti, tvrdosť a lomová húževnatosť. Za pozitívny výsledok možno považovať, že ani prísada 10 hmot.% oxidov vzácnych zemín nezhoršila mechanické vlastnosti pri izbovej teplote, naopak napr. lomová húževnatosť materiálov dokonca vzrástla. Výrazný rozdiel medzi vplyvom rôznych prvkov vzácnych zemín na spekanie a mechanické vlastnosti materiálov pri izbovej teplote nebol pozorovaný. Tieto prísady sú pridávané za

účelom zlepšenia vysokoteplotných vlastností, akými sú odolnosť materiálov proti oxidácii a ablácii. Tieto vlastnosti budú študované v nasledujúcom kroku, pričom sa očakáva výrazný vplyv množstva a typu oxidu prvku vzácnej zeme. Počas riešenia projektu sa taktiež skúmala možnosť tvorby usporiadaných štruktúr u diboridových keramik. Ako modelový systém sa študoval materiál na báze TiB₂ a tiež kompozitný systém TiB₂-SiC. K usporiadaniu, resp. textúre došlo vplyvom pôsobenia silného magnetického poľa počas odlievania keramickej suspenzie obsahujúcej požadované chemické zloženie. Bolo jasne preukázané, že texturované materiály majú výrazne zlepšené mechanické vlastnosti v jednom smere. V ďalšom kroku sa bude skúmať možnosť texturovania komplexnej, viacfázovej štruktúry s prídavkom prvkov vzácnych zemín.

Výstupy:

1. TATARKO, Peter - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra – MEDVEĎ Dávid - DLOUHÝ, Ivo - REECE, Michael J. Highly textured and strongly anisotropic TiB₂ ceramics prepared using magnetic field alignment (9T), In Journal of the European Ceramic Society, 2019, in press, <https://doi.org/10.1016/j.jeurceramsoc.2019.11.006>.
2. FÜRDÖSOVÁ, Zuzana - ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - TATARKO, Peter. ZrB₂-SiC ceramics with rare-earth oxide additives. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic: book of extended abstracts. Ed. Jana Valúchová; 2019, p. 57-61. ISBN 978-80-971648-8-1.
3. TATARKO, Peter - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - REECE, Michael J. Preparation of highly textured TiB₂-based ceramics using a strong magnetic field. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019: book of abstracts, 2019, p. 51. ISBN 978-80-971648-7-4.
4. FÜRDÖSOVÁ, Zuzana - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - DLOUHÝ, Ivo - TATARKO, Peter. Influence of powder processing route and rare earth additives on the mechanical properties of ZrB₂-SiC ceramics. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019: abstract book. - Italy, 2019, p. 813.
5. FÜRDÖSOVÁ, Zuzana - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - DLOUHÝ, Ivo - TATARKO, Peter. Preparation and characterization of ZrB₂-based ceramics with rare earth oxide additives. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019: book of abstracts, p. 71. ISBN 978-80-971648-7-4.
6. ÜNSAL, Hakan - SHEPA, Ivan - HANZEL, Ondrej - MÚDRA, Erika - VOJTKO, Marek - DUSZA, Ján - TATARKO, Peter. In situ synthesis and characterization of B₄C-TiB₂ fibers composites. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019: abstract book. - Italy, 2019, p. 701.

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:	1 - Slovensko: 1
Čerpané financie:	APVV: 27100 €

Dosiahnuté výsledky:

V prvej etape riešenia projektu boli pripravené hutné materiály na báze Si₃N₄ s rôznymi spekáciami prísadami na báze kremičitanov a fosforečnanov. Bol optimalizovaný proces teploty a času spekania s cieľom dosiahnuť na hraniciach nitridu kremičitého bioaktívne fázy. Analýzou kryštalických fáz pomocou röntgenovej difrakcie a amorfných fáz energiovo disperznou analýzou boli vybrané spekacie prísady, ktorých vplyv na výsledné mechanické vlastnosti (tvrdosť, pevnosť) a biologickú odozvu bude študovaný v nasledujúcich etapách projektu.

Výstupy:

HÍČÁK, Michal - HNATKO, Miroslav - LABUDOVÁ, Martina - GALUSKOVÁ, Dagmar - SEDLÁČEK, Jaroslav - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol. Bioproperties of Si₃N₄-based ceramics after oxy-acetylene flame treatment = Biologické vlastnosti keramiky na báze Si₃N₄ po opracovaní povrchu kyslíkovo-acetylénovým plameňom. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic: book of extended abstracts. - Bratislava, Slovak Republic: Institute of Inorganic Chemistry SAS, 2019, p. 30-41. ISBN 978-80-971648-8-1. (Workshop Processing and properties of advanced ceramics and glasses).
TATARKOVÁ, Monika - TATARKO, Peter - DLOUHÝ, Ivo - DUSZA, Ján. Sintering behaviour and microstructural

evolution of silicon nitride composites with boron nitride platelets. In Preparation of ceramic materials: Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. Košice: Technical University, 2019, p. 111-114. ISBN 978-80-553-3314-4.

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: 9867 €

Dosiahnuté výsledky:

V rámci podaktivity 1.4. sme sa venovali modifikácii povrchu mikroguličiek na báze nitridu kremičitého s prídavkom bioaktívnej zložky (tzv. bioaktívne plnivo) za účelom skúmania zmien ich biologických vlastností. Rovnako sme sa začali venovať príprave hutných keramických materiálov pre extrémne aplikácie na báze boridov a karbidov ako aj príprave kompozitov s prídavkom grafénu.

HIČÁK, Michal - HNATKO, Miroslav - LABUDOVÁ, Martina - GALUSKOVÁ, Dagmar - SEDLÁČEK, Jaroslav - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol. Bioproperties of Si₃N₄-based ceramics after oxy-acetylene flame treatment = Biologické vlastnosti keramiky na báze Si₃N₄ po opracovaní povrchu kyslíkovo-acetylenovým plameňom. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic: book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Micháľková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic: Institute of Inorganic Chemistry SAS, 2019, p. 30-41. ISBN 978-80-971648-8-1.

ŠIMKO, František - RAKHMATULLIN, Aydar - VÉRON, Emmanuel - ALLIX, Mathieu - FLORIAN, Pierre - KORENKO, Michal - NETRIOVÁ, Zuzana - BESSADA, Catherine. Oxo- and (oxo)(fluoro)-aluminates: Synthesis, stability and structure correlation = Oxo- a (oxo)(fluoro)-hlinitany: Syntézy, stabilita a vzájomná štruktúrna korelácia. In Interakce tavenin s progresivními anorganickými materiály, 10. odborný seminář, 14. - 15. října 2019, Hradec nad Moravicí, Česká republika. - Česká republika: VŠB TU Ostrava, 2019, p. 11-13.

HANZEL, Ondrej - SINGH, Meinam Annebushan - MARLA, Deepak - SEDLÁK, Richard - ŠAJGALÍK, Pavol. Wire electrical discharge machinable SiC with GNPs and GO as the electrically conducting filler. In Journal of the European Ceramic Society, 2019, vol. 39, no. 8, p. 2626-2633. (4.029 - IF2018). ISSN 0955-2219.

Príloha C - Publikačná činnosť organizácie (generovaná z ARL)**ADCA Vedecké práce v zahraničných karentovaných časopisoch – impaktovaných**

- ADCA01 BAČÍK, Peter** - FRIDRICHOVÁ, Jana - UHER, Pavel - RYBÁR, S. - KUREKOVÁ, Valéria - LUPTÁKOVÁ, Jarmila - VRABLÍKOVÁ, Dana - PUKANČÍK, Libor - VACULOVÍČ, T. Octahedral substitution in beryl from weakly fractionated intragranitic pegmatite Predne Solisko, Tatry Mountains (Slovakia): the indicator of genetic conditions. In Journal of Geosciences, 2019, vol. 64, no. 1, p. 59-72. (2018: 1.275 - IF, Q3 - JCR, 0.559 - SJR, Q2 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 1802-6222.
- ADCA02 BOČA, Miroslav** - NETRIOVÁ, Zuzana - RAKHMATULLIN, Aydar - VASKOVÁ, Zuzana - HADZIMOVÁ, Eva - SMRČOK, Ľubomír - HANZEL, Ondrej - KUBÍKOVÁ, Blanka. The differing responses of various techniques in measuring the phase transformations of K₂ZrF₆. In Journal of Molecular Liquids, 2019, vol. 287, p. 110969-1-110969-10. (2018: 4.561 - IF, Q1 - JCR, 0.862 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0167-7322.
- ADCA03 BORA, Pankaj L. - NOVOTNÝ, Jan - RUUD, Kenneth - KOMOROVSKÝ, Stanislav - MAREK, Radek**. Electron-spin structure and metal-ligand bonding in open-shell systems from relativistic EPR and NMR: A case study of square-planar iridium catalysts. In Journal of Chemical Theory and Computation, 2019, vol. 15, no. 1, p. 201-214. (2018: 5.313 - IF, Q1 - JCR, 2.236 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 1549-9618.
- ADCA04 CASTRO, Abril C. - FLIEGL, Heike - CASCELLA, Michele - HELGAKER, Trygve - REPISKÝ, Michal - KOMOROVSKÝ, Stanislav - ÁNGELES MEDRANO, María - QUIROGA, Adoración G. - SWART, Marcel**. Four-component relativistic 31P NMR calculations for trans-platinum(II) complexes: importance of the solvent and dynamics in spectral simulations. In Dalton Transactions, 2019, vol. 48, no. 23, p. 8076-8083. (2018: 4.052 - IF, Q1 - JCR, 1.120 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 1477-9226.
- ADCA05 DASAN, A. - ELSAYED, H. - KRAXNER, Jozef - GALUSEK, Dušan - BERNARDO, E.**. Hierarchically porous 3D-printed akermanite scaffolds from silicones and engineered fillers. In Journal of the European Ceramic Society, 2019, vol. 39, no. 14, p. 4445-4449. (2018: 4.029 - IF, Q1 - JCR, 1.219 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0955-2219.
- ADCA06 DUAN, Yusen** - ZHANG, Jingxian** - LI, Xiaoguang - BAI, Hainan - ŠAJGALÍK, Pavol - JIANG, Dongliang. High thermal conductivity silicon nitride ceramics prepared by pressureless sintering with ternary sintering additives. In International Journal of Applied Ceramic Technology, 2019, vol. 16, no. 4, p. 1399-1406. (2018: 1.074 - IF, Q2 - JCR, 0.371 - SJR, Q2 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 1744-7402.
- ADCA07 DŽUNDA, Róbert** - FIDES, Martin - HNATKO, Miroslav - HVIŽDOŠ, Pavol - MÚDRA, Erika - MEDVEĎ, Dávid - KOVALČÍKOVÁ, Alexandra - MILKOVIČ, Ondrej. Mechanical, physical properties and tribological behaviour of silicon carbide composites with addition of carbon nanotubes. In International Journal of Refractory Metals and Hard Materials, 2019, vol. 81, p. 272-280. (2018: 2.794 - IF, Q1 - JCR, 1.062 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0263-4368.
- ADCA08 ELSAYED, H. - PICICCO, Martiniano - DASAN, A. - KRAXNER, Jozef - GALUSEK, Dušan - BERNARDO, E.**. Glass powders and reactive silicone binder: Interactions and application to additive manufacturing of bioactive glass-ceramic scaffolds. In Ceramics International, 2019, vol. 45, no. 11, p. 13740-13746. (2018: 3.450 - IF, Q1 - JCR, 0.888 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0272-8842.
- ADCA09 GAÁLOVÁ, Barbora - VYLETELOVÁ, Ivana - POKORNÁ, Katarína - KIKHNEY, Judith - MONET, Annette - BUJDÁK, Juraj - BUJDÁKOVÁ, Helena**. Decreased vitality and viability of Escherichia coli isolated by adherence to saponite particles. In Applied Clay Science, 2019, vol. 183, p. 105316-1-105316-9. (2018: 3.890 - IF, Q1 - JCR, 0.990 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0169-1317.
- ADCA10 HANZEL, Ondrej** - SINGH, Meinam Annebushan - MARLA, Deepak - SEDLÁK, Richard - ŠAJGALÍK, Pavol. Wire electrical discharge machinable SiC with GNPs and GO as the electrically conducting filler. In Journal of the European Ceramic Society, 2019, vol. 39, no. 8, p. 2626-2633. (2018: 4.029 - IF, Q1 - JCR, 1.219 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0955-2219.
- ADCA11 HRUŠKA, Branislav** - NETRIOVÁ, Zuzana - VASKOVÁ, Zuzana - BOČA, Miroslav - CHROMČÍKOVÁ, Mária - LIŠKA, Marek. High-temperature Raman study of K₂ZrF₆ phase transitions. In Journal of Alloys and Compounds, 2019, vol. 791, p. 45-50. (2018: 4.175 - IF, Q1 - JCR, 1.065 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0925-8388.
- ADCA12 HRUŠKA, Branislav** - OSIPOV, Armenak A. - OSIPOVA, Leyla M. - CHROMČÍKOVÁ, Mária -

- MACHÁČEK, Jan. Thermodynamic model and Raman spectra of BaO-B₂O₃ glasses. In *Vibrational Spectroscopy*, 2019, vol. 105, p. 102970-1-102970-5. (2018: 1.861 - IF, Q3 - JCR, 0.440 - SJR, Q3 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0924-2031.
- ADCA13 CHEHAIBOU, Bilal - BADAWI, Michael - BUČKO, Tomáš - BAZHIROV, Timur - ROCCA, Dario**. Computing RPA adsorption enthalpies by machine learning thermodynamic perturbation theory. In *Journal of Chemical Theory and Computation*, 2019, vol. 15, no. 11, p. 6333-6342. (2018: 5.313 - IF, Q1 - JCR, 2.236 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 1549-9618.
- ADCA14 CHROMČÍKOVÁ, Mária** - OSIPOV, Armenak A. - OSIPOVA, Leyla M. - HRUŠKA, Branislav - LIŠKA, Marek - SVOBODA, Roman. Thermodynamic model and high temperature Raman spectra of Na₂O-B₂O₃ glassforming melts. In *Journal of Alloys and Compounds*, 2019, vol. 798, p. 700-705. (2018: 4.175 - IF, Q1 - JCR, 1.065 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0925-8388.
- ADCA15 KOMOROVSKÝ, Stanislav** - CHERRY, Peter - REPISKÝ, Michal. Four-component relativistic time-dependent density-functional theory using a stable noncollinear DFT ansatz applicable to both closed- and open-shell systems. In *Journal of Chemical Physics*, 2019, vol. 151, no. 18, p. 184111-1-184111-14. (2018: 2.997 - IF, Q2 - JCR, 1.159 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0021-9606.
- ADCA16 KONEČNÝ, Lukáš** - REPISKÝ, Michal - RUUD, Kenneth - KOMOROVSKÝ, Stanislav**. Relativistic four-component linear damped response TDDFT for electronic absorption and circular dichroism calculations. In *Journal of Chemical Physics*, 2019, vol. 151, no. 19, p. 194112-1-194112-14. (2018: 2.997 - IF, Q2 - JCR, 1.159 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0021-9606.
- ADCA17 KORENKO, Michal** - ŠIMKO, František - MLYNÁRIKOVÁ, Jarmila - LARSON, Carol - MIKŠÍKOVÁ, Eva - PRIŠČÁK, Jozef - AMBROVÁ, Marta - PALUMBO, Robert. Physico-chemical properties of (MgF₂-CaF₂-(LiF))eut-MgO system as a molten electrolyte for Mg electrowinning. In *Journal of Molecular Liquids*, 2019, vol. 275, p. 535-543. (2018: 4.561 - IF, Q1 - JCR, 0.862 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0167-7322.
- ADCA18 KOTULOVÁ, Júlia** - STAREK, Dušan - HAVELCOVÁ, Martina - PÁLKOVÁ, Helena. Amber and organic matter from the late Oligocene deep-water deposits of the Central Western Carpathians (Orava-Podhale Basin). In *International Journal of Coal Geology*, 2019, vol. 207, p. 96-109. (2018: 5.330 - IF, Q1 - JCR, 2.333 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0166-5162.
- ADCA19 KRAXNER, Jozef** - MICHÁLEK, Martin - ROMERO, Acacio R. - ELSAYED, H. - BERNARDO, E. - BOCCACCINI, Aldo - GALUSEK, Dušan. Porous bioactive glass microspheres prepared by flame synthesis process. In *Materials Letters*, 2019, vol. 256, p. 126625-1-126625-4. (2018: 3.019 - IF, Q2 - JCR, 0.771 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0167-577X.
- ADCA20 KUREKOVÁ, Valéria - BELUŠÁKOVÁ, Silvia - BOHÁČ, Peter - BUJDÁK, Juraj**. Resonance energy transfer in the systems of smectite modified with a fluorescent cationic polymer and a photosensitizer. In *Applied Clay Science*, 2019, vol. 183, no., p. 105326-1-105326-9. (2018: 3.890 - IF, Q1 - JCR, 0.990 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0169-1317.
- ADCA21 LACKOVIČOVÁ, Monika - BARANYAIOVÁ, Tímea - BUJDÁK, Juraj**. The chemical stabilization of methylene blue in colloidal dispersions of smectites. In *Applied Clay Science*, 2019, vol. 181, no., p. 105222-1-105222-8. (2018: 3.890 - IF, Q1 - JCR, 0.990 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0169-1317.
- ADCA22 MARLTAN, W. - VENKATESWARA RAO, P.** - TEKIN, H.O. - SAYYED, M.I.** - KLEMENT, Róbert - GALUSEK, Dušan - LAKSHMINARAYANA, G. - SYAM PRASAD, P. - VEERAAIAH, N. Analysis of red mud doped Bi₂O₃-B₂O₃-BaO glasses for application as glass solder in radiation shield repair using MCNPX simulation. In *Ceramics International*, 2019, vol. 45, no. 6, p. 7619-7626. (2018: 3.450 - IF, Q1 - JCR, 0.888 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0272-8842.
- ADCA23 MARLTAN, W. - VENKATESWARA RAO, P.** - KLEMENT, Róbert - GALUSEK, Dušan - SAYYED, M.I. - TEKIN, H.O. - SYAM PRASAD, P. - VEERAAIAH, N. Spectroscopic and thermal analysis of lead-free multipurpose radiation shielding glasses. In *Ceramics International*, 2019, vol. 45, no. 5, p. 5332-5338. (2018: 3.450 - IF, Q1 - JCR, 0.888 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0272-8842.
- ADCA24 NERÁD, Ivan - MIKŠÍKOVÁ, Eva - KUBÍKOVÁ, Blanka**. Calorimetric investigation of tripotassium zirconate heptafluoride K₃ZrF₇. In *Journal of Molecular Liquids*, 2019, vol. 290, p. 111191-1-111191-3. (2018: 4.561 - IF, Q1 - JCR, 0.862 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0167-7322.
- ADCA25 OSIPOV, Armenak A.** - OSIPOVA, Leyla M. - HRUŠKA, Branislav - OSIPOV, Artem A. - LIŠKA, Marek. FTIR and Raman spectroscopy studies of ZnO-doped BaO.2B₂O₃ glass mix. In *Vibrational Spectroscopy*, 2019, vol. 103, p. 102921-1-102921-7. (2018: 1.861 - IF, Q3 - JCR, 0.440 - SJR, Q3 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0924-2031.

- ADCA26 PASTOREK, Adam - HRNČÍŘOVÁ, Jana - JANKOVIČ, Ľuboš - NEJDL, Lukáš - CIVIŠ, Svatopluk - IVANEK, Ondřej - SHESTIVSKA, Violetta - KNÍŽEK, Antonín - KUBELÍK, Petr - ŠPONER, Jiří - PETERA, Lukáš - KŘIVKOVÁ, Anna - CASSONE, Guiseppe - VACULOVIČOVÁ, Markéta** - ŠPONER, Judit E.** - FERUS, Martin**. Prebiotic synthesis at impact craters: the role of Fe-clays and iron meteorites. In Chemical Communication, 2019, vol. 55, no. 71, p. 10563-10566. (2018: 6.164 - IF, Q1 - JCR, 2.177 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 1359-7345.
- ADCA27 PETŘÍKOVÁ, I.** - PARCHOVIANSKÝ, Milan - ŠVANČÁREK, Peter - LENZ LEITE, Mateus - MOTZ, Günter - GALUSEK, Dušan. Passive filler loaded polysilazane-derived glass/ceramic coating system applied to AISI 441 stainless steel, part 1: Processing and characterization. In International Journal of Applied Ceramic Technology, 2019, vol. (2018: 1.074 - IF, Q2 - JCR, 0.371 - SJR, Q2 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 1744-7402.
- ADCA28 POLOVOV, Ilya B.** - BATAEV, Ya. S. - AFONIN, Yu. D. - VOLKOVICH, Vladimir - CHUKIN, Andrey V. - RAKHMATULLIN, Aydar - BOČA, Miroslav. Synthesis of HfO₂ from hafnium hydroxide hydrate. In Journal of Alloys and Compounds, 2019, vol. 790, p. 405-412. (2018: 4.175 - IF, Q1 - JCR, 1.065 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0925-8388.
- ADCA29 REY, Jérôme - GOMEZ, Axel - RAYBAUD, Pascal - CHIZALLET, Céline** - BUČKO, Tomáš**. On the origin of the difference between type A and type B skeletal isomerization of alkanes catalyzed by zeolites: The crucial input of ab initio molecular dynamics. In Journal of Catalysis, 2019, vol. 373, p. 361-373. (2018: 7.723 - IF, Q1 - JCR, 2.254 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0021-9517.
- ADCA30 REY, Jérôme - RAYBAUD, Pascal - CHIZALLET, Céline** - BUČKO, Tomáš**. Competition of secondary versus tertiary carbenium routes for the type B isomerization of alkenes over acid zeolites quantified by ab initio molecular dynamics simulations. In ACS Catalysis, 2019, vol. 9, no. 11, p. 9813-9828. (2018: 12.221 - IF, Q1 - JCR, 4.702 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 2155-5435.
- ADCA31 ROCCA, Dario** - DIXIT, Anant - BADAWI, Michael - LEBÈGUE, Sébastien - GOULD, Tim - BUČKO, Tomáš**. Bridging molecular dynamics and correlated wave-function methods for accurate finite-temperature properties. In Physical Review Materials, 2019, vol. 3, no. 4, art. no. 040801, p. 1-6. (2018: 2.926 - IF, Q2 - JCR, karentované - CCC). (2019 - Current Contents). ISSN 2475-9953.
- ADCA32 SHEN, Lingling - ZHAO, Bo - ZHANG, Baoguo - XU, Junli - BOČA, Miroslav - SHI, Zhongning**. Preparation and characterization of amorphous Cr₂O₃ nanoparticles obtained by solution plasma discharge. In Ceramics International, 2019, vol. 45, no. 17, p. 23578-23585. (2018: 3.450 - IF, Q1 - JCR, 0.888 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0272-8842.
- ADCA33 SHEN, Lingling - KONG, Lingqiang - ZHAO, Bo - FENG, Sen - LIU, Aimin - XU, Junli - BOČA, Miroslav - SHI, Zhongning**. Formation of NiO and Ni in an aqueous solution using plasma discharge electrolysis. In Journal of the Electrochemical Society, 2019, vol. 166, no. 12, p. e365-e374. (2018: 3.120 - IF, Q1 - JCR, 1.138 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0013-4651.
- ADCA34 SCHOLTZOVÁ, Eva** - TUNEGA, Daniel. Density functional theory study of the stability of the tetrabutylphosphonium and tetrabutylammonium montmorillonites. In Clay Minerals, 2019, vol. 54, no. 1, p. 41-48. (2018: 1.787 - IF, Q3 - JCR, 0.415 - SJR, Q3 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0009-8558.
- ADCA35 SLANÝ, Michal** - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana. Structural characterization of organo-montmorillonites prepared from a series of primary alkylamines salts: Mid-IR and near-IR study. In Applied Clay Science, 2019, vol. 176, p. 11-20. (2018: 3.890 - IF, Q1 - JCR, 0.990 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0169-1317.
- ADCA36 SVOBODA, Roman** - MÁLEK, Jiří - LIŠKA, Marek. Correlation between the structure and structural relaxation data for (GeSe₂)_y(Sb₂Se₃)_{1-y} glasses. In Journal of Non-Crystalline Solids, 2019, vol. 505, p. 162-169. (2018: 2.600 - IF, Q1 - JCR, 0.689 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0022-3093.
- ADCA37 SVOBODA, Roman** - BRANDOVÁ, Daniela - CHROMČÍKOVÁ, Mária - LIŠKA, Marek. Thermokinetic behavior of Ga-doped GeTe₄ glasses. In Journal of Non-Crystalline Solids, 2019, vol. 512, p. 7-14. (2018: 2.600 - IF, Q1 - JCR, 0.689 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0022-3093.
- ADCA38 TALIMIAN, Ali** - GALUSEK, Dušan. Aqueous slip casting of translucent magnesium aluminate spinel: Effects of dispersant concentration and solid loading. In Ceramics International, 2019, vol. 45, no. 6, p. 10646-10653. (2018: 3.450 - IF, Q1 - JCR, 0.888 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0272-8842.
- ADCA39 TALIMIAN, Ali** - POUCHLÝ, Václav - EL-MAGHRABY, Hesham F. M. Aldelrehim - MACA, Karel - GALUSEK, Dušan. Impact of high energy ball milling on densification behaviour of magnesium aluminate spinel evaluated by master sintering curve and constant rate of heating approach.

- In Ceramics International, 2019, vol. 45, no. 17, p. 23467-23474. (2018: 3.450 - IF, Q1 - JCR, 0.888 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents, WOS, SCOPUS). ISSN 0272-8842.
- ADCA40 VARGA, Peter** - UHLÍK, Peter* - LEXA, Jaroslav - ŠURKA, Juraj - KUREKOVÁ, Valéria - HUDEC, Pavol - PÁLKOVÁ, Helena. The influence of porosity on the release of water from perlite glass. In Monatshefte für Chemie, 2019, vol. 150, no. 6, p. 1025-1040. (2018: 1.501 - IF, Q3 - JCR, 0.337 - SJR, Q2 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0026-9247.
- ADCA41 VOKELOVÁ, Jana - MICHÁLKOVÁ, J. - CHROMČÍKOVÁ, Mária - HRUŠKA, Branislav - LIŠKA, Marek**. Leaching kinetics of IZOMER TT glass fibrous insulation. In Ceramics-Silikáty, 2019, vol. 63, no. 3, p. 287-290. (2018: 0.840 - IF, Q3 - JCR, 0.352 - SJR, Q2 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 0862-5468.
- ADCA42 WISNIEWSKI, Wolfgang** - ŠVANČÁREK, Peter - PARCHOVIANSKÝ, Milan - THIEME, Christian - RÜSSEL, Christian. Hindering the kinetic selection of dendritic Ba-fresnoite by phase separation in a glass of the near-eutectic composition Ba₂TiSi₂O₈-2.625SiO₂. In Crystal Growth & Design, 2019, vol. 19, no. 6, p. 3559-3566. (2018: 4.153 - IF, Q1 - JCR, 1.046 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 1528-7483.
- ADCA43 ZIMOWSKA, Malgorzata** - GURGUL, J. - SCHOLTZOVÁ, Eva - SOCHA, Robert P. - PÁLKOVÁ, Helena - LITYNSKA-DOBRYNSKA, L. - MORKZYCKI, Lukasz - LATKA, K. A precursor approach for the development of lace-like Fe₂O₃ nanocrystallites triggered by pressure dependent nucleation and growth of akaganeite over clay based composites for toluene combustion. In Journal of Physical Chemistry C, 2019, vol. 123, no. 43, p. 26236-26250. (2018: 4.309 - IF, Q1 - JCR, 1.652 - SJR, Q1 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 1932-7447.

ADDA Vedecké práce v domácich karentovaných časopisoch – impaktovaných

- ADDA01 OSACKÝ, Marek** - BINČÍK, Tomáš - PAĽO, Tomáš - UHLÍK, Peter - MADEJOVÁ, Jana - CZÍMEROVÁ, Adriana. Mineralogical and physico-chemical properties of bentonites from the Jastrabá Formation (Kremnické vrchy Mts., Western Carpathians). In Geologica Carpathica, 2019, vol. 70, no. 5, p. 433-445. (2018: 1.699 - IF, Q3 - JCR, 0.627 - SJR, Q2 - SJR, karentované - CCC). (2019 - Current Contents). ISSN 1335-0552.

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

- ADMA01 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.
- ADMA02 SINGH, Meinam Annebushan** - RAJBONGSHI, Sanjib Kr - SARMA, Deba Kumar - HANZEL, Ondrej - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Surface and porous recast layer analysis in μ -EDM of MWCNT-Al₂O₃ 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.

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

- ADMB01 KITYK, A. ** - PROTSENKO, V. - PAVLÍK, Viliam - BOČA, Miroslav. Corrosion resistance of AISI 304 and AISI 316 stainless steels in a solar salt used in concentrated solar power plants: The effect of NaCl impurities. In Voprosy khimii i khimicheskoi tekhnologii, 2019, no. 3, p. 123-131. (2018: 0.131 - SJR, Q4 - SJR). ISSN 0321-4095.
- ADMB02 KITYK, A. ** - KUN, O. - PAVLÍK, Viliam - BOČA, Miroslav. Electropolishing of stainless steel with a high content of manganese in the deep eutectic mixture Ethaline. In Voprosy khimii i khimicheskoi tekhnologii, 2019, no. 6, p. 92-98. (2018: 0.131 - SJR, Q4 - SJR). ISSN 0321-4095.

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

- ADNB01 MAJEROVÁ, Melinda - ŠKRÁTEK, Martin - PRNOVÁ, Anna - DVUREČENSKI, Andrej - KRAXNER, Jozef - ŠVANČÁREK, Peter - CIGÁŇ, Alexander - MAŇKA, Ján - GALUSEK, Dušan. Preparation and characterization of Ni doped Ca₂Al₂SiO₇ glass microspheres. In MEASUREMENT 2019: Proceedings of the 12th International Conference on Measurement. - Bratislava, Slovakia : Institute of Measurement Science, Slovak Academy of Sciences, 2019, p. 282-285. ISBN 978-80-

972629-2-1.

AFA Publikované pozvané príspevky na zahraničných vedeckých konferenciách

- AFA01 PRNOVÁ, Anna - VALÚCHOVÁ, Jana - DOHNALOVÁ ŽANETA - HANZEL, Ondrej - KLEMENT, Róbert - BRUNEEL, E. - GALUSEK, Dušan. Preparation of Al₂O₃-Y₂O₃ glass microspheres; influence of particle size distribution on thermal behavior of prepared systems. In Konferencie o speciálných anorganických pigmentech a práškových materiáloch, 18. září 2019, Pardubice : sborník příspěvků 21. ročníku. Z odp. redaktor Žaneta Dohnalová, Petra Šulcová. - Pardubice, Česká republika : Univerzita Pardubice, 2019, p.44-47. ISBN 978-80-7560-222-0.(Konferencie o speciálných anorganických pigmentech a práškových materiáloch).

AFC Publikované príspevky na zahraničných vedeckých konferenciách

- AFC01 HANZEL, Ondrej - LENČEŠ, Zoltán - KIM, Young-Wook - FEDOR, Ján - ŠAJGALÍK, Pavol. Electrical and thermal conductivity of SiC-graphene composites annealed in nitrogen atmosphere = Elektrická a tepelná vodivosť kompozitov SiC-grafén žíhaných v atmosfére dusíka. In Interakce tavenin s progresivními anorganickými materiály, 10. odborný seminář, 14. - 15. října 2019, Hradec nad Moravicí, Česká republika. - Česká republika : VŠB TU Ostrava, 2019, p. 4-10.(Interakce tavenin s progresivními anorganickými materiály).
- AFC02 HRUŠKA, Branislav - CHROMČÍKOVÁ, Mária - MICHÁLKOVÁ, J. - VOKELOVÁ, Jana - LIŠKA, Marek. Identifikácia povrchovo aktívnych zložiek sklotvornej taveniny pomocou termodynamického modelu = Surface active components of glassforming melts identified by thermodynamic model. In 41. Mezinárodní český a slovenský kalorimetrický seminář : Sborník příspěvků. Z odp. red. Zdeněk Černošek, Jana Holubová, Eva Černošková ; recenzenti Pavla Rovnaníková, Václav Švorčík, Zdeňka Kolská, František Hnilička. - Pardubice : Univerzita Pardubice, 2019, p. 81-84. ISBN 977-80-7560-213-8.(Mezinárodní český a slovenský kalorimetrický seminář).
- AFC03 CHROMČÍKOVÁ, Mária - DAGUPATI, Rajesh - MUNOZ, F. - HRUŠKA, Branislav - MICHÁLKOVÁ, J. - LIŠKA, Marek. Selected thermomechanical properties of binary barium-phosphate glasses = Vybrané termomechanické vlastnosti binárnych bárnato-fosforečnanových skiel. In 41. Mezinárodní český a slovenský kalorimetrický seminář : Sborník příspěvků. Z odp. red. Zdeněk Černošek, Jana Holubová, Eva Černošková ; recenzenti Pavla Rovnaníková, Václav Švorčík, Zdeňka Kolská, František Hnilička. - Pardubice : Univerzita Pardubice, 2019, p. 65-68. ISBN 977-80-7560-213-8.(Mezinárodní český a slovenský kalorimetrický seminář).
- AFC04 MICHÁLKOVÁ, J. - VOKELOVÁ, Jana - CHROMČÍKOVÁ, Mária - HRUŠKA, Branislav - LIŠKA, Marek. Chemická odolnosť sklovláknitej izolácie NUKON používanej v jadrových elektrárňach = Chemical durability of NUKON glass fibrous insulation used in nuclear power plants. In 41. Mezinárodní český a slovenský kalorimetrický seminář : Sborník příspěvků. Z odp. red. Zdeněk Černošek, Jana Holubová, Eva Černošková ; recenzenti Pavla Rovnaníková, Václav Švorčík, Zdeňka Kolská, František Hnilička. - Pardubice : Univerzita Pardubice, 2019, p. 99-102. ISBN 977-80-7560-213-8.(Mezinárodní český a slovenský kalorimetrický seminář).
- AFC05 ŠIMKO, František - RAKHMATULLIN, Aydar - VÉRON, Emmanuel - ALLIX, Mathieu - FLORIAN, Pierre - KORENKO, Michal - NETRIOVÁ, Zuzana - BESSADA, Catherine. Oxo- and (oxo)(fluoro)-aluminates: Synthesis, stability and structure correlation = Oxo- a (oxo)(fluoro)-hlinitaný: Syntézy, stabilita a vzájomná štruktúrna korelácia. In Interakce tavenin s progresivními anorganickými materiály, 10. odborný seminář, 14. - 15. října 2019, Hradec nad Moravicí, Česká republika. - Česká republika : VŠB TU Ostrava, 2019, p. 11-13.(Interakce tavenin s progresivními anorganickými materiály).
- AFC06 VOKELOVÁ, Jana - MICHÁLKOVÁ, J. - CHROMČÍKOVÁ, Mária - LIŠKA, Marek - HRUŠKA, Branislav. Kinetika korózie sklenených vlákien IZOMER TT v kvapalných médiách = Kinetics of corrosion of glass fibers IZOMER TT in liquid media. In 41. Mezinárodní český a slovenský kalorimetrický seminář : Sborník příspěvků. Z odp. red. Zdeněk Černošek, Jana Holubová, Eva Černošková ; recenzenti Pavla Rovnaníková, Václav Švorčík, Zdeňka Kolská, František Hnilička. - Pardubice : Univerzita Pardubice, 2019, p. 111-114. ISBN 977-80-7560-213-8.(Mezinárodní český a slovenský kalorimetrický seminář).

AFD Publikované príspevky na domácich vedeckých konferenciách

- AFD01 AKUSEVICH, A. - PARCHOVIANSKÁ, I. - PARCHOVIANSKÝ, Milan - PRNOVÁ, Anna - KLEMENT, Róbert. Preparation of Ce³⁺-doped phosphors by sintering of glass microspheres - preliminary study = Príprava Ce³⁺-dopovaných luminoforov spekaním sklenených mikrogulôčok - predbežné štúdium. In Workshop Processing and properties of advanced ceramics and glasses,

- November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Michálková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 117-125. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD02 BYSTRICKÝ, Roman - HNATKO, Miroslav - SEDLÁČEK, Jaroslav. Preparation of lightweight aggregates from industrial waste. In Preparation of ceramic materials : Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. - Košice : Technical University, 2019, p. 33-37. ISBN 978-80-553-3314-4.(Preparation of ceramic materials : international conference).
- AFD03 FÜRDÖSOVÁ, Zuzana - ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - TATARKO, Peter. ZrB₂-SiC ceramics with rare-earth oxide additives = Keramické materiály na báze ZrB₂-SiC s prísadami oxidov prvkov vzácnych zemín. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Michálková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 57-61. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD04 GALUSKOVÁ, Dagmar - KAŇKOVÁ, Hana - ŠVANČÁRKOVÁ, Anna - GALUSEK, Dušan. Assesment of ion release at early stage of immersion in SB fluid for novel biomaterials = Posúdenie počiatkovej fázy rozpúšťania novodobých biomateriálov v SB kvapaline. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Michálková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 26-29. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD05 GOVINDAN, Nibu Putenpurayil - MICHÁLKOVÁ, Monika - GALUSEK, Dušan. Ce³⁺ doped yttria nanopowders for transparent yttria ceramics prepared by precipitation method. In Preparation of ceramic materials : Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. - Košice : Technical University, 2019, p. 133-139. ISBN 978-80-553-3314-4.(Preparation of ceramic materials : international conference).
- AFD06 HÍČÁK, Michal - HNATKO, Miroslav - LABUDOVÁ, Martina - GALUSKOVÁ, Dagmar - SEDLÁČEK, Jaroslav - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol. Bioproperties of Si₃N₄-based ceramics after oxy-acetylene flame treatment = Biologické vlastnosti keramiky na báze Si₃N₄ po opracovaní povrchu kyslíkovo-acetylenovým plameňom. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Michálková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 30-41. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD07 HNATKO, Miroslav - HÍČÁK, Michal - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Surface modification of dense silicon nitride. In Preparation of ceramic materials : Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. - Košice : Technical University, 2019, p. 103-109. ISBN 978-80-553-3314-4.(Preparation of ceramic materials : international conference).
- AFD08 KLEMENT, Róbert - DRDLÍKOVÁ, K. - DRDLÍK, Daniel - MACA, Karel - GALUSEK, Dušan. Analysis of optical properties of Al₂O₃:Cr³⁺ polycrystalline transparent red light emitting ceramics = Analýza optických vlastností Al₂O₃:Cr³⁺ polykryštalickej transparentnej keramiky emitujúcej červené svetlo. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Michálková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 102-112. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD09 KRAXNER, Jozef - MICHÁLEK, Martin - ROMERO, Acacio R. - ELSAIED, H. - BERNARDO, E. - GALUSEK, Dušan. Porous bioactive glass microspheres prepared by flame synthesis = Pórovité bioaktívne sklené mikrogulôčky pripravené plameňovou syntézou. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Michálková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. čl'-čý. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD10 LENČEŠ, Zoltán - PETRISKOVÁ, Patrícia - RADWAN, Mohamed - HNATKO, Miroslav. Spinel-based ceramic materials for LED and photocatalytic applications. In ALER 2019. Medzinárodná vedecko-odborná konferencia Alternatívne zdroje energie, 2. - 4. 10. 2019, Závažná Poruba, Slovakia

- : proceedings. Editor Pavel Šimon. - Liptovský Mikuláš, 2019, p. 76-81. ISBN 978-80-89456-36-9.(ALER 2019. Medzinárodná vedecko-odborná konferencia Alternatívne zdroje energie - Alternative Energy Resources).
- AFD11 MAJEROVÁ, Melinda - PRNOVÁ, Anna - KLEMENT, Róbert - ŠKRÁTEK, Martin - CIGÁŇ, Alexander - DVUREČENSKIJ, Andrej - ŠVANČÁREK, Peter - KRAXNER, Jozef - MAŇKA, Ján - GALUSEK, Dušan. Ni-doped gehlenite glass microspheres: preparation and characterization = Ni-dopované gelenitové sklené mikrogulôčky: príprava a charakterizácia. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Micháľková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 126-135. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD12 MEDVECKÝ, Ľubomír - ŠTULAJTEROVÁ, Radoslava - GIRETOVÁ, Mária - SOPČÁK, Tibor - HNATKO, Miroslav - FENCLOVÁ, Taťána. Properties and microstructure of calcium phosphate cement composite containing Si₃N₄ microgranules. In Preparation of ceramic materials : Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. - Košice : Technical University, 2019, p. 186-187. ISBN 978-80-553-3314-4.(Preparation of ceramic materials : international conference).
- AFD13 MICHÁLEK, Martin - KURTULDU, F. - NEŠČÁKOVÁ, Z. - LIVERANI, L. - GALUSEK, Dušan - BOCCACCINI, Aldo. Mesoporous bioactive glass doped with therapeutic ions = Mezoporézne bioaktívne sklá dopované terapeutickými iónmi. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Micháľková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 22-25. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD14 MICHÁLKOVÁ, Monika - KRAXNER, Jozef - POUCHLÝ, Václav - MACA, Karel - GALUSEK, Dušan. Spark plasma sintering of glass microspheres with YAG composition = Spekanie skla so zložením hlinito-yttritého granátu pomocou SPS. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Micháľková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 113-116. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD15 PARCHOVIANSKÝ, Milan - PARCHOVIANSKÁ, I. - ŠVANČÁREK, Peter - MOTZ, Günter - GALUSEK, Dušan. Preparation and corrosion behaviour of PDC layers with passive fillers = Príprava a korózia keramických vrstiev pripravených z organokremičitých prekursorov s pasívnymi plnivami. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Micháľková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 79-83. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD16 ŠVANČÁREK, Peter - KLEMENT, Róbert - PARCHOVIANSKÝ, Milan - GALUSEK, Dušan. White light emitting Y₂O₃ based fluorecents doped with ZnO = Biele svetlo emitujúce fluorecenty na báze Y₂O₃ dopovaného pomocou ZnO. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Micháľková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 96-101. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD17 TATARKO, Peter - ZHOU, Xiaobing - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo. Joining of SiC ceramics with Ti-based alloys by SPS. P. Tatarko, X. Zhou, A. Kovalčíková, I. Dlouhý. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Micháľková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 68-72. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).
- AFD18 TATARKOVÁ, Monika - TATARKO, Peter - DLOUHÝ, Ivo - DUSZA, Ján. Sintering behaviour and microstructural evolution of silicon nitride composites with boron nitride platelets. In Preparation of ceramic materials : Proceedings of the 13th international conference. Jahodná, 25.-27.6.2019. Eds. B. Plešingerová, D. Medved'. - Košice : Technical University, 2019, p. 111-114. ISBN 978-80-553-3314-4.(Preparation of ceramic materials : international conference).
- AFD19 ÜNSAL, Hakan - SHEPA, Ivan - MATOVIC, Branko - HANZEL, Ondrej - MÚDRA, Erika -

TATARKO, Peter. Densification of B4C-TiB2 composites by field assisted sintering = Príprava B4C-TiB2 kompozitov spekaním za asistencie elektrického prúdu. In Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Micháľková, Jozef Ráhel', Peter Tatarko. - Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019, p. 52-56. ISBN 978-80-971648-8-1.(Workshop Processing and properties of advanced ceramics and glasses).

AFE Abstrakty pozvaných príspevkov zo zahraničných konferencií

- AFE01 BOČA, Miroslav - ŠIMURDA, Michal - ŠVEC, Peter - ŠVEC, Peter Jr. - JANIČKOVIČ, Dušan - CZÍMEROVÁ, Adriana - KUBÍKOVÁ, Blanka - MLYNÁRIKOVÁ, Jarmila. Unexpected phase transformations in ternary fluoride systems. In 19th European Symposium on Fluorine Chemistry : Book of Abstracts. - Warszawa, Poland : Oficyna Wydawnicza-Poligraficzna ADAM, 2019, p. 134.
- AFE02 CHROMČÍKOVÁ, Mária - HRUŠKA, Branislav - LIŠKA, Marek. Získavanie hodnotných dát analýzou nevydarených termolátometrických experimentov. In TAS 2019. Termoanalytický seminár, 10. říjen 2019, Brno : sborník příspěvků. Z odp. redaktori Petra Šulcová, Václav Slovák. - Brno, Česká republika : Česká společnost chemická, z.s., 2019, s. 9-11. ISBN 978-80-88307-03-7.(TAS 2019. Termoanalytický seminár).
- AFE03 KOMOROVSKÝ, Stanislav - CHERRY, Peter - REPISKÝ, Michal. Relativistic theory for prediction of excitation energies of both closed- and open-shell species. In CESTC 2019. 17th Central European Symposium on Theoretical Chemistry, 9th - 12th September, 2019, Burg Schlaining, Austria : book of abstracts. - Austria, 2019, p. 17.(CESTC 2019. Central European Symposium on Theoretical Chemistry).
- AFE04 ŠAJGALÍK, Pavol - HNATKO, Miroslav - KAŠIAROVÁ, Monika - SEDLÁČEK, Jaroslav - BYSTRICKÝ, Roman - LENČEŠ, Zoltán - GALUSKOVÁ, Dagmar. Corrosion of silicon nitride and alumina based ceramics by molten iron. In REFRA PRAGUE 2019 : book of abstracts. - Prague, Czech Republic : Silikátová společnost ČR, 2019, p. 4. ISBN 978-80-02-02861-1.(REFRA PRAGUE 2019).
- AFE05 ŠAJGALÍK, Pavol. New nitrides and carbides for high temperature application. In ICCT. 7th International Conference on Chemical Technology, 15. - 17. 4. 2019, Mikulov, Czech Republic : book of abstracts. - Czech Republic, 2019, 1 p. ISBN 978-80-88307-01-3. Názov z obrazovky. Požaduje sa Adobe Acrobat Reader.

AFF Abstrakty pozvaných príspevkov z domácich konferencií

- AFF01 BALESTRAT, M. - LALE, A. - HANZEL, Ondrej - LENČEŠ, Zoltán - BERNARD, Samuel. Dense silicon carbide and silicon nitride-based ceramics with high electrical conductivity via precursor chemistry. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. Eds. Zoltán Lenčéš, Jana Valúchová. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 37. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFF02 BERNARDO, E. - ELSAYED, H. - DASAN, A. - KRAXNER, Jozef - GALUSEK, Dušan. Silicones and engineered fillers: from crystalline silicate ceramics to glass-ceramics. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. Eds. Zoltán Lenčéš, Jana Valúchová. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 26. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFF03 MACA, Karel - DRDLÍKOVÁ, K. - SPUSTA, Tomáš - DRDLÍK, Daniel - KLEMENT, Róbert - GALUSEK, Dušan. Processing and properties of photoluminescent transparent polycrystalline alumina ceramics prepared by hot isostatic pressing. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. Eds. Zoltán Lenčéš, Jana Valúchová. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 29. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFF04 MALKIN, Vladimír - MALKINA, Olga. Calculations and interpretation of the EPR parameters in the framework of 2- and 4-component DFT approach. In XIth EFEPR 2019 Conference : book of abstracts. - Bratislava : Vydavateľstvo SCHK, 2019, pL6, 1 p. ISBN 978-80-8208-020-2.
- AFF05 ZHOU, Xiaobing - TATARKO, Peter - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - HUANG, Z. - HUANG, Q. SiC ceramics joined with an in-situ reaction gradient layer of TiC/Ti3SiC2 using electric field-assisted sintering technique. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. Eds. Zoltán Lenčéš, Jana Valúchová. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 52. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).

AFG Abstrakty príspevkov zo zahraničných konferencií

- AFG01 HRUŠKA, Branislav - DAGUPATI, Rajesh - CHROMČÍKOVÁ, Mária - VOKELOVÁ, Jana - LIŠKA, Marek - MUNOZ, F. Thermodynamic model and raman spectra of BaO-P2O5 glasses. In 2nd Journal of Thermal Analysis and Calorimetry Conference, Budapest, Hungary, June 18-21, 2019 : book of abstracts. - Hungary, 2019, p. 405-406. ISBN 978-963-454-416-6.(Journal of Thermal Analysis and Calorimetry Conference).
- AFG02 HRUŠKA, Branislav - DAGUPATI, Rajesh - CHROMČÍKOVÁ, Mária - MACHÁČEK, Jan - LIŠKA, Marek - MUNOZ, F. Thermodynamic model and Raman spectra of MgO-P2O5 glasses. In CEEC-TAC5 & Medicta2019. 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry (CEEC-TAC5) and 14th Mediterranean Conference on Calorimetry and Thermal Analysis (Medicta2019) : book of abstracts. - Germany : Central and Eastern European Committee for Thermal Analysis and Calorimetry, 2019, p. 478. ISBN 978-3-940237-59-0.(CEEC-TAC5 & MEDICTA 2019 : 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry and 14th Mediterranean Conference on Calorimetry and Thermal Analysis).
- AFG03 CHODÁK, Ivan - JOCHEC MOŠKOVÁ, Daniela - JANIGOVÁ, Ivica - JANKOVIČ, Ľuboš - KRONEK, Juraj - OMASTOVÁ, Mária. Properties of poly(epsilon-caprolactone)/clay nanocomposites. In EUROFILLERS 2019 : POLYMER BLENDS : 50 years of Polymer Research at the University of Palermo : in honour of retirement of Prof. Francesco Paolo La Mantia [elektronický zdroj]. - Palermo, Italy: University of Palermo, 2019, [2] p. Názov z obrazovky. Požaduje sa Adobe Acrobat Reader DC(EUROFILLERS 2019 : POLYMER BLENDS : 50 years of Polymer Research at the University of Palermo : in honour of the retirement of Prof. Francesco Paolo La Mantia).
- AFG04 CHROMČÍKOVÁ, Mária - OSIPOV, Armenak A. - OSIPOVA, Leyla M. - HRUŠKA, Branislav - MICHÁLKOVÁ, J. - LIŠKA, Marek. Thermodynamic model and high-temperature raman spectra of BaO-B2O3 glassforming melts. In 2nd Journal of Thermal Analysis and Calorimetry Conference, Budapest, Hungary, June 18-21, 2019: book of abstracts. - Hungary, 2019, p. 398-399. ISBN 978-963-454-416-6.(Journal of Thermal Analysis and Calorimetry Conference).
- AFG05 CHROMČÍKOVÁ, Mária - DAGUPATI, Rajesh - SVOBODA, Roman - HRUŠKA, Branislav - LIŠKA, Marek - MUNOZ, F. Structure and volume relaxation of selected BaO-P2O5 glasses. In CEEC-TAC5 & Medicta2019. 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry (CEEC-TAC5) and 14th Mediterranean Conference on Calorimetry and Thermal Analysis (Medicta2019) : book of abstracts. - Germany: Central and Eastern European Committee for Thermal Analysis and Calorimetry, 2019, p. 474. ISBN 978-3-940237-59-0.(CEEC-TAC5 & MEDICTA 2019 : 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry and 14th Mediterranean Conference on Calorimetry and Thermal Analysis).
- AFG06 KODĚRA, Peter - TAKÁCS, Ágnes - RACEK, Martin - ŠIMKO, František - LUPTÁKOVÁ, Jarmila - VÁCZI, Tamás - ANTAL, Peter. Javoriete - the type mineral of shallow porphyry gold systems, hosted by salt melt inclusions. In Acta Mineralogica-Petrographica : Abstract Series. - Szeged : Department of Mineralogy, Geochemistry and Petrology, University of Szeged, 2019, vol. 10, p. 60. ISSN 1589-4835.(ECROFI XXV).
- AFG07 MAJEROVÁ, Melinda - PRNOVÁ, Anna - PLŠKO, Alfonz - ŠVANČÁREK, Peter - VALÚCHOVÁ, Jana - KLEMENT, R. - GALUSEK, Dušan. Crystallization kinetics of gehlenite glass microspheres. In 2nd Journal of Thermal Analysis and Calorimetry Conference (JTACC 2019) : Book of Abstracts. - Hungary, 2019, p. 410. ISBN 978-963-454-416-6.(Journal of Thermal Analysis and Calorimetry Conference).
- AFG08 MAJEROVÁ, Melinda - PRNOVÁ, Anna - PLŠKO, Alfonz - HRUŠKA, B. - VALÚCHOVÁ, Jana - KRAXNER, J. - BRUNEEL, E. - GALUSEK, Dušan. Crystallization kinetics of Ni-doped Ca2Al2SiO7 glass microspheres. In CEEC-TAC5 & Medicta2019. 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry (CEEC-TAC5) and 14th Mediterranean Conference on Calorimetry and Thermal Analysis (Medicta2019) : book of abstracts. - Germany : Central and Eastern European Committee for Thermal Analysis and Calorimetry, 2019, p. 479. ISBN 978-3-940237-59-0.(CEEC-TAC5 & MEDICTA 2019 : 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry and 14th Mediterranean Conference on Calorimetry and Thermal Analysis).
- AFG09 PLŠKO, Alfonz - PAGÁČOVÁ, Jana - PAPUČOVÁ, Iveta - PRNOVÁ, Anna - VALÚCHOVÁ, Jana - HRUŠKA, Branislav - ONDRUŠOVÁ, D. Crystallization of TiO2 xerogel. In CEEC-TAC5 & Medicta2019. 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry (CEEC-TAC5) and 14th Mediterranean Conference on Calorimetry and Thermal Analysis (Medicta2019) : book of abstracts. - Germany: Central and Eastern European Committee for Thermal Analysis and Calorimetry, 2019, p. 481. ISBN 978-3-940237-59-0.(CEEC-TAC5 & MEDICTA 2019 : 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry and 14th Mediterranean Conference on Calorimetry and Thermal Analysis).
- AFG10 PRNOVÁ, Anna - PLŠKO, Alfonz - VALÚCHOVÁ, Jana - KLEMENT, Róbert - CHROMČÍKOVÁ,

- AFG11 Mária - MAJEROVÁ, Melinda - BRUNEEL, E. - GALUSEK, Dušan. Crystallization kinetics of binary Yb₂O₃-Al₂O₃ glass. In CEEC-TAC5 & Medicta2019. 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry (CEEC-TAC5) and 14th Mediterranean Conference on Calorimetry and Thermal Analysis (Medicta2019) : book of abstracts. - Germany: Central and Eastern European Committee for Thermal Analysis and Calorimetry, 2019, p. 475. ISBN 978-3-940237-59-0.(CEEC-TAC5 & MEDICTA 2019 : 5th Central and Eastern European Conference on Thermal Analysis and Calorimetry and 14th Mediterranean Conference on Calorimetry and Thermal Analysis).
- AFG12 SHEPA, Ivan - MÚDRA, Erika - VOJTKO, Marek - TATARKO, Peter - DUSZA, Ján. Nanoceramic materials by needle-less electrospinning. In NANO 2019: International research and practice conference "NANOTECHNOLOGY AND NANOMATERIALS", Book of abstracts, 27-30 August 2019, Lviv, Ukraine. - Lviv, Ukraine: Computer-publishing, information center, 2019, p. 142. ISBN 978-966-97587-3-6.
- TATARKO, Peter - VALENZA, Fabrizio - ÜNSAL, Hakan - KOVALČÍKOVÁ, Alexandra - BYSTRICKÝ, Roman. Wetting and phase interaction between Cf/SiC and transition metal disilicides-based alloys. In HT-CMC10. 10th International conference on high temperature ceramic matrix composites, September 22-26, 2019, Bordeaux, France : book of abstracts. - France, 2019, p. 323.(HT-CMC10. International Conference on High Temperature Ceramic Matrix Composites).

AFH Abstrakty príspevkov z domácich konferencií

- AFH01 BARANYAIOVÁ, Tímea - BUJDÁK, Juraj - SEBECHLEBSKÁ, Táňa - ŠIMON, Erik. Molecular aggregation of xanthene dye in colloidal dispersions of layered silicate: The effect of ionic strength. In 6th Workshop of Slovak Clay Group: Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia: Slovak Clay Group, 2019, p. 1-2. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH02 BARLOG, Martin - PÁLKOVÁ, Helena - BUJDÁK, Juraj. Spectral properties of hybrid systems based on organomodified smectites and rhodamine 6G. In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 3-4. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH03 BELUŠÁKOVÁ, Silvia - BUJDÁK, Juraj - MARTÍNEZ-MARTÍNEZ, Virginia - SOLA-LLANO, R. - LOPEZ ARBELOA, I. FRET and Poisson distance distribution model as the tools for the characterization of the dye surface concentration on the smectite particles. In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 5. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH04 BOČA, Miroslav - ŠIMURDA, Michal - ŠVEC, Peter - ŠVEC, Peter Jr. - JANIČKOVIČ, Dušan - CZÍMEROVÁ, Adriana - KUBÍKOVÁ, Blanka - NETRIOVÁ, Zuzana - MLYNÁRIKOVÁ, Jarmila. Unusual phase transformations in ternary fluoride systems. In ChemZi : Zborník abstraktov: 71. Zjazd chemikov, 9-13 september 2019, Vysoké Tatry, Horný Smokovec, Slovensko. - Bratislava : Slovenská chemická spoločnosť, 2019, roč. 15, č. 1, s. 82. ISSN 1336-7242.
- AFH05 BUJDÁK, Juraj - BARANYAIOVÁ, Tímea. What do we know about the mechanism of dye molecular aggregation in colloids of inorganic nanoparticles? In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 6-7. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH06 BYSTRICKÝ, Roman - ŠKRÁTEK, Martin - SEDLÁČEK, Jaroslav - RUSNÁK, Jaroslav - ŠAJGALÍK, Pavol. Electrical and magnetic properties of SiC with Ti and NbC as sintering aids. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 67. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH07 EL-MAGHRABY, Hesham F. M. Aldelrehim - SEDLÁČEK, Jaroslav - KACHLÍK, M. - SPUSTA, Tomáš - MACA, Karel - GALUSEK, Dušan. Solid-state fabrication of transparent YAG ceramics for optical applications: Characterization, mixing, and processing of the starting oxides. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 28. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH08 FRIDRICHOVÁ, Jana - BAČÍK, Peter - UHER, Pavel - RYBÁR, S. - BIZOVSKÁ, Valéria - LUPTÁKOVÁ, Jarmila - VRABLÍKOVÁ, Dana - PUKANČÍK, Libor - VACULOVIČ, T. Beryl from weakly fractionated granitic pegmatite Predné Solisko, Tatry Mountains (Slovakia): Octahedral

- substitution as the indicator of environmental conditions. In Mineralogicko-petrologická konferencia Petros 2019 : Zborník recenzovaných abstraktov a príspevkov. - Bratislava : Univerzita Komenského v Bratislave vo Vydavateľstve UK, 2019, p. 20. ISBN 978-80-223-4713-6.(Petros 2019).
- AFH09 FÜRDÖSOVÁ, Zuzana - KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - DLOUHÝ, Ivo - TATARKO, Peter. Preparation and characterization of ZrB₂-based ceramics with rare earth oxide additives. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 71. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH10 HANZEL, Ondrej - SINGH, Meinam Annebushan - MARLA, Deepak - SEDLÁK, Richard - ŠAJGALÍK, Pavol. Electro-discharge machinable SiC-graphene composites. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 38. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH11 HNATKO, Miroslav - HICÁK, Michal - LABUDOVÁ, Martina - GALUSKOVÁ, Dagmar - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Modification of biocompatible dense silicon nitride to bioactive ceramics by surface oxidation. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 73. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH12 KAŠIAROVÁ, Monika - HNATKO, Miroslav - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - ŠAJGALÍK, Pavol. Preparation and mechanical properties of silicone nitride-hydroxyapatite composite scaffolds. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 84. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH13 KOVÁČOVÁ, Zuzana - BAČA, Ľuboš - NEUBAUER, Erich - SEDLÁČEK, Jaroslav - OROVČÍK, Ľubomír - DOBROČKA, Edmund - KITZMANTEL, M. Synthesis of ZrB₂ using YSZ and oxidation behavior of its composites with SiC up to 2000 °C. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 76. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH14 KOVALČÍKOVÁ, Alexandra - HANZEL, Ondrej - SEDLÁK, Richard - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol - DUSZA, Ján. Tribological properties of differently oriented graphene platelets in silicon carbide/graphene composites. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 77. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH15 KOVALČÍKOVÁ, Alexandra - TATARKO, Peter - MEDVEĎ, Dávid - SEDLÁK, Richard - CHLUP, Zdeněk - MÚDRA, Erika - DUSZA, Ján. Effect of graphene platelets on mechanical and tribological properties of TiB₂-SiC-GPLs ceramic composites. In Fractography of advanced ceramics FAC 2019 : The International conference. Book of abstracts. Smolenice, 8.-11.9.2019. - Košice : Institute of Materials Research SAS, 2019, p. no. ISBN 978-80-89782-12-3.(Fractography of advanced ceramics FAC 2019 : The international conference).
- AFH16 KUBÍKOVÁ, Blanka - MLYNÁRIKOVÁ, Jarmila - MIKŠÍKOVÁ, Eva - BOČA, Miroslav. Physico-chemical properties of molten lanthanide systems. In ChemZi : Zborník abstraktov: 71. Zjazd chemikov, 9-13 september 2019, Vysoké Tatry, Horný Smokovec, Slovensko. - Bratislava : Slovenská chemická spoločnosť, 2019, 2019, roč. 15, č. 1, s. 170. ISSN 1336-7242.
- AFH17 KUREKOVÁ, Valéria - PÁLKOVÁ, Helena - MADEJOVÁ, Jana - VARGA, Peter - LEXA, Jaroslav - UHLÍK, Peter. New approach to the determination of water in perlitites by infrared methods. In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 9-10. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH18 LENČEŠ, Zoltán - CZÍMEROVÁ, Adriana - PETRISKOVÁ, Patrícia - KLEMENT, Róbert - HULMAN, Martin. Influence of lanthanide oxides and fluorides on the photoluminescence of LaSi₃N₅. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 79. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH19 LENZ LEITE, Mateus - DEGENHARDT, Ulrich - KRENKEL, Walter - GALUSEK, Dušan - MOTZ, Günter. Environmental barrier coatings based on ytterbium oxide and oligosilazanes for protection of Si₃N₄. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice

- castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 56. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH20 MADEJOVÁ, Jana. Near-IR spectroscopy and organoclays. In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 11-12. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH21 MALKINA, Oľga - MALKIN, Vladimír. Visualization of relativistic effects on EPR hyperfine coupling pathways. In XIth EFEPR 2019 Conference : book of abstracts. - Bratislava : Vydavateľstvo SCHK, 2019, p.39, 1p. ISBN 978-80-8208-020-2.
- AFH22 MICHÁLKOVÁ, Monika - KRAXNER, Jozef - GALUSEK, Dušan. Preparation of translucent YAG glass/ceramic at temperature below 900 °C. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 30. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH23 MORENO RODRÍGUEZ, Daniel - SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - TUNEGA, Daniel. Density functional theory study of atrazine-beidellite intercalates. In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 13-14. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH24 PÁLKOVÁ, Helena - HRONSKÝ, Viktor - KUREKOVÁ, Valéria - MADEJOVÁ, Jana. The influence of the organic cation on the water uptake by clay minerals: Spectroscopic study. In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 15-16. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH25 PETRISKOVÁ, Patrícia - RADWAN, Mohamed - MONFORT, O. - PLESCH, Gustáv - LENČEŠ, Zoltán. Photocatalytic TiO₂ nanotubes arrays formation on polymeric and ceramic substrates. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 81. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH26 PODHRADSKÁ, Silvia - PEIDAYESH, Hamed - MOSNÁČKOVÁ, Katarína - JOCHEC MOŠKOVÁ, Daniela - JANKOVIČ, Ľuboš - CHODÁK, Ivan. Properties of poly(epsilon-caprolactone)/clay nanocomposites. In BYPoS : conference book. - Bratislava : Young Scientist Council of Polymer Institute SAS, 2019, p. 72. ISBN 978-80-89841-09-7.(BYPoS 2019 : Bratislava Young Polymer Scientists conference).
- AFH27 PUCHÝ, Viktor - IVOR, Michal - MEDVEĎ, Dávid - HNATKO, Miroslav - KOVALČÍKOVÁ, Alexandra - HVIZDOŠ, Pavol. Preparation, friction, wear, and fracture of the Si₃N₄-Ag-GNPs composites prepared by SPS. In Fractography of advanced ceramics FAC 2019 : The International conference. Book of abstracts. Smolenice, 8.-11.9.2019. - Košice : Institute of Materials Research SAS, 2019, p. no. ISBN 978-80-89782-12-3.(Fractography of advanced ceramics FAC 2019 : The international conference).
- AFH28 SEDLÁČEK, Jaroslav - HNATKO, Miroslav - LÁZÁR, Marián - ČARNOGURSKÁ, M. - BRESTOVIČ, Tomáš. Processing and thermal properties of porous glass-ceramics from waste. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 82. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH29 SCHOLTZOVÁ, Eva. Computational study of Cs-hectorite. In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 17-18. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH30 SLANÝ, Michal - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana. Modern methods of IR spectroscopy and their utilization for conformation study of alkylammonium cations intercalated in montmorillonites. In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 19-20. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH31 ŠAJGALÍK, Pavol. Micro-cantilever testing of Si₃N₄ based ceramics with different sintering additives.

- In Fractography of advanced ceramics FAC 2019 : The International conference. Book of abstracts. Smolenice, 8.-11.9.2019. - Košice : Institute of Materials Research SAS, 2019, 1 p. ISBN 978-80-89782-12-3.(Fractography of advanced ceramics FAC 2019 : The international conference).
- AFH32 ŠIMKO, František - RAKHMATULLIN, Aydar - VÉRON, Emmanuel - ALLIX, Mathieu - FLORIAN, Pierre - BUČKO, Tomáš - NETRIOVÁ, Zuzana - KORENKO, Michal - BESSADA, Catherine. Fluoro-, oxo- and oxofluoro-aluminates: Synthesis, and their stability. In ChemZi : Zborník abstraktov: 71. Zjazd chemikov, 9-13 september 2019, Vysoké Tatry, Horný Smokovec, Slovensko. - Bratislava : Slovenská chemická spoločnosť, 2019, 2019, roč. 15, č. 1, s. 174. ISSN 1336-7242.
- AFH33 ŠKORŇA, Peter - SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - TUNEGA, Daniel. Structural and spectroscopic characterization of beidellite intercalated with choline and acetylcholine. In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 21-22. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH34 TALIMIAN, Ali - POUCHLY, V. - EL-MAGHRABY, Hesham F. M. Abdelrehim - MACA, Karel - GALUSEK, Dušan. Sintering of magnesium aluminate spinel doped with MnF₂ and CoF₂. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 32. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH35 TATARKO, Peter - GRASSO, Salvatore - KOVALČÍKOVÁ, Alexandra - DLOUHÝ, Ivo - REECE, Michael J. Preparation of highly textured TiB₂-based ceramics using a strong magnetic field. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 51. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).
- AFH36 TATARKOVÁ, Monika - TATARKO, Peter - DLOUHÝ, Ivo - DUSZA, Ján. Mechanical properties of Si₃N₄ with BN nanoplatelets prepared by SPS. In Fractography of advanced ceramics FAC 2019 : The International conference. Book of abstracts. Smolenice, 8.-11.9.2019. - Košice : Institute of Materials Research SAS, 2019, p. no. ISBN 978-80-89782-12-3.(Fractography of advanced ceramics FAC 2019 : The international conference).
- AFH37 UHLÍK, Peter - KUBAČ, Alexander - SZCZERBA, M. - BIRON, Adrián - KODĚRA, Peter - MILOVSKÝ, Rastislav - OSACKÝ, Marek - PÁLKOVÁ, Helena. Illite - Indicator of hydrothermal alteration conditions in epithermal deposit Banská Hodruša. In 6th Workshop of Slovak Clay Group : Clay minerals and selected non-raw materials in material science, industrial applications and environmental technology. May 27-28, 2019, Banská Bystrica, Slovakia : book of abstracts. - Bratislava, Slovakia : Slovak Clay Group, 2019, p. 23. ISBN 978-80-972367-3-1.(Workshop of Slovak Clay Group).
- AFH38 ÜNSAL, Hakan - SHEPA, Ivan - HANZEL, Ondrej - MÚDRA, Erika - VOJTKO, Marek - DUSZA, Ján - TATARKO, Peter. The effect of temperature and pressure on the densification behaviour of B₄C-TiB₂(f) composites. In Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. - Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019, p. 85. ISBN 978-80-971648-7-4.(Engineering Ceramics 2019 : Ceramics for people).

FAI Zostavovateľské práce knižného charakteru (bibliografie, encyklopédie, katalógy, slovníky, zborníky, atlasy ...)

- FAI01 Workshop Processing and properties of advanced ceramics and glasses, November 20-22, 2019, Ráztočno, Slovak Republic : book of extended abstracts. Ed. Jana Valúchová; recenzenti Marián Janek, Robert Klement, Alexandra Kovalčíková, Monika Michálková, Jozef Ráhel, Peter Tatarko. Bratislava, Slovak Republic : Institute of Inorganic Chemistry SAS, 2019. 149 p. ISBN 978-80-971648-8-1(Workshop Processing and properties of advanced ceramics and glasses).
- FAI02 Engineering Ceramics 2019, Advanced Research Workshop: Ceramics for people, Smolenice castle, May 12-16, 2019 : book of abstracts. Eds. Zoltán Lenčes, Jana Valúchová. Bratislava, Slovakia : Institute of Inorganic Chemistry, Slovak Academy of Sciences, 2019. 91 p. ISBN 978-80-971648-7-4(Engineering Ceramics 2019 : Ceramics for people).

GII Rôzne publikácie a dokumenty, ktoré nemožno zaradiť do žiadnej z predchádzajúcich kategórií

- GII01 BABU, S. - PLŠKO, Alfonz - GALUSEK, Dušan - CASTRO, Y. - DURÁN, A. Fabrication of transparent and nanostructured doped and undoped NaGdF₄ glass-ceramic coatings for optoelectronic

- device applications. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 765.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII02 BARANYAIOVÁ, Tímea - BUJDÁK, Juraj - SEBECHLEBSKÁ, Táňa. Effect of ionic strength on the molecular aggregation of cationic dye in colloidal dispersions with montmorillonite particles. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 112.(EUROCLAY 2019. International conference on clay science and technology).
- GII03 BARLOG, Martin - PÁLKOVÁ, Helena - BUJDÁK, Juraj. Spectroscopic study of organo-smectites and cationic laser dye hybrid systems. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 113.(EUROCLAY 2019. International conference on clay science and technology).
- GII04 BELUŠÁKOVÁ, Silvia - SOLA-LLANO, R. - LOPEZ ARBELOA, I. - MARTÍNEZ-MARTÍNEZ, Virginia - BUJDÁK, Juraj. Resonance energy transfer between dye molecules in hybrid films of a layered silicate including the effect of dye surface concentration. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 123.(EUROCLAY 2019. International conference on clay science and technology).
- GII05 BERTOLLA, Luca - CHLUP, Zdeněk - TATARKO, Peter - HANZEL, Ondrej - ŠEVEČEK, Oldřich - ROUPCOVÁ, Pavla - DLOUHÝ, Ivo. Composite Al₂O₃/SiO₂/CaO foams reinforced with cellulose acetate fibers from cigarette tows. In CICC-11 : The Eleventh International Conference on High-Performance Ceramics, May 25-29, 2019, Kunming, China : abstract book. - China : The Chinese Ceramic Society, 2019, p. 345.(CICC-11 : International Conference on High-Performance Ceramics).
- GII06 BERTOLLA, Luca - ŠEVEČEK, Oldřich - DLOUHÝ, Ivo - TATARKO, Peter. Composite Al₂O₃/SiO₂/CaO foams reinforced with cellulose acetate fibres from cigarette tows. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 27.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII07 BOČA, Miroslav - ŠIMURDA, Michal - ŠVEC, Peter - ŠVEC, Peter Jr. - JANIČKOVIČ, Dušan - CZÍMEROVÁ, Adriana - KUBÍKOVÁ, Blanka - MLYNÁRIKOVÁ, Jarmila. Unusual phase transformations in ternary fluoride systems. In MS11. 11th international symposium on molten salts - chemistry and technology, 19-23 Mai 2019, Orleans, France : program and abstracts. - France, 2019, p. 87.(MS11. International symposium on molten salts - chemistry and technology).
- GII08 BOHÁČ, Peter - CZÍMEROVÁ, Adriana - SASAI, Ryo - BUJDÁK, Juraj. Hybrid systems based on layered silicate and cyanine dyes prepared by LBL method for studying FRET phenomenon. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 134.(EUROCLAY 2019. International conference on clay science and technology).
- GII09 BUJDÁK, Juraj - BARANYAIOVÁ, Tímea - SEBECHLEBSKÁ, Táňa. On the mechanism of molecular aggregation of dyes in colloidal dispersions of clay minerals. The effect of temperature. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 149.(EUROCLAY 2019. International conference on clay science and technology).
- GII10 DASAN, A. - ELSAYED, H. - KRAXNER, Jozef - GALUSEK, Dušan - BERNARDO, E. Hierarchically porous 3D-printed Åkermanite scaffolds from silicones and engineered fillers. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 42.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII11 FÜRDÖSOVÁ, Zuzana - KOVALČIKOVÁ, Alexandra - HANZEL, Ondrej - DLOUHÝ, Ivo - TATARKO, Peter. Influence of powder processing route and rare earth additives on the mechanical properties of ZrB₂-SiC ceramics. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 813.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII12 GALUSEK, Dušan - TALIMIAN, Ali - POUCHLÝ, Václav - EL-MAGHRABY, Hesham F. M. Abdelrehim - MACA, Karel. Transparent magnesium aluminate spinel: Effect of critical temperature in two-stage spark plasma sintering. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 487.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII13 HANZEL, Ondrej - LENČEŠ, Zoltán - KIM, Young-Wook - ŠAJGALÍK, Pavol. Silicon carbide-graphene composites with high functional properties sintered by direct hot-press. In CICC-11 : The Eleventh International Conference on High-Performance Ceramics, May 25-29, 2019, Kunming, China : abstract book. - China : The Chinese Ceramic Society, 2019, p. 55-56.(CICC-11 : International Conference on High-Performance Ceramics).
- GII14 HANZEL, Ondrej - LENČEŠ, Zoltán - KIM, Young-Wook - ŠAJGALÍK, Pavol. Silicon carbide-graphene composites with high electrical and thermal conductivity. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 270.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII15 HNATKO, Miroslav - LÁZÁR, Marián - SEDLÁČEK, Jaroslav - ČARNOGURSKÁ, M. -

- BRESTOVIČ, Tomáš. Glass-ceramic foam - usability of vitrified waste from plasma smelting process. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 870.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII16 JANKOVIČ, Ľuboš - KRONEK, Juraj - MADEJOVÁ, Jana - HRONSKÝ, Viktor. Intercalation of montmorillonite with functionalized surfactant. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 322.(EUROCLAY 2019. International conference on clay science and technology).
- GII17 JANKOVIČ, Ľuboš. Sorption an textile dye to clay modified with phosphonium surfactants. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 321.(EUROCLAY 2019. International conference on clay science and technology).
- GII18 KORENKO, Michal - ŠIMKO, František - MLYNÁRIKOVÁ, Jarmila - LARSON, Carol - MIKŠÍKOVÁ, Eva - PRIŠČÁK, Jozef - PALUMBO, Robert - AMBROVÁ, Marta. Physico-chemical properties of (MgF₂-CaF₂-(LiF))eut-MgO system as a molten electrolyte for solar thermal Mg electrowinning. In MS11. 11th international symposium on molten salts - chemistry and technology, 19-23 Mai 2019, Orleans, France : program and abstracts. - France, 2019, p. 58.(MS11. International symposium on molten salts - chemistry and technology).
- GII19 KOVÁČOVÁ, Zuzana - BAČA, Ľuboš - NEUBAUER, Erich - SEDLÁČEK, Jaroslav - OROVČÍK, Ľubomír - KITZMANTEL, M. Characterization and oxidation behaviour of YB₄ and its composites. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 816.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII20 KOVALČÍKOVÁ, Alexandra - TATARKO, Peter - SEDLÁK, Richard - MEDVEĎ, Dávid - HÚLAN, Michal - MÚDRA, Erika - IVOR, Michal - DUSZA, Ján. Mechanical and tribological properties of TiB₂-SiC-GPLs ceramic composites. In CICC-11 : The Eleventh International Conference on High-Performance Ceramics, May 25-29, 2019, Kunming, China : abstract book. - China : The Chinese Ceramic Society, 2019, p. 86.(CICC-11 : International Conference on High-Performance Ceramics).
- GII21 KRAXNER, Jozef - DASAN, A. - ELSAYED, H. - BERNARDO, E. - GALUSEK, Dušan. Combining flame synthesis and additive manufacturing technology for the preparation of novel Åkermanite scaffolds. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 371.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII22 KUBÍKOVÁ, Blanka - MLYNÁRIKOVÁ, Jarmila - BOČA, Miroslav. Physico-chemical properties of molten lanthanide systems. In MS11. 11th international symposium on molten salts - chemistry and technology, 19-23 Mai 2019, Orleans, France : program and abstracts. - France, 2019, p. 91.(MS11. International symposium on molten salts - chemistry and technology).
- GII23 LENČEŠ, Zoltán - RADWAN, Mohamed - ŠAJGALÍK, Pavol. Preparation of transparent MgAl₂O₄ ceramics for LED applications. In ICACC 2019. 43rd International Conference & Exposition on Advanced Ceramics and Composites, January 27 - February 1, 2019, Daytona Beach, Florida, USA : abstract book. - USA : The American Ceramic Society, 2019, p. 36.(ICACC 2019. International Conference & Exposition on Advanced Ceramics and Composites).
- GII24 LENČEŠ, Zoltán - RADWAN, Mohamed - CZÍMEROVÁ, Adriana - ŠAJGALÍK, Pavol. Preparation of transparent/translucent spinel-based phosphors. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 507.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII25 MACA, Karel - DRDLÍKOVÁ, K. - SPUSTA, Tomáš - DRDLÍK, Daniel - KLEMENT, Róbert - GALUSEK, Dušan. Transparent structural and functional alumina ceramics prepared by pressure-less presintering and hot isostatic pressing. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 161.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII26 MADEJOVÁ, Jana - KOMADEL, Peter - PÁLKOVÁ, Helena. Infrared spectroscopy in studies of acid-treated clay minerals. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 411.(EUROCLAY 2019. International conference on clay science and technology).
- GII27 MORENO RODRÍGUEZ, Daniel - SCHOLTZOVA, Eva - JANKOVIČ, Ľuboš - TUNEGA, Daniel. Atrazine-Montmorillonite/Beidellite intercalates: a density functional theory study. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 456.(EUROCLAY 2019. International conference on clay science and technology).
- GII28 OSACKÝ, Marek - VÍTKOVÁ, Martina - JANKOVIČ, Ľuboš - CZÍMEROVÁ, Adriana - PÁLKOVÁ, Helena - HUDEC, Pavol - SEDLÁČEK, Jaroslav. Role of mineralogy, chemistry and surface properties of different zeolitic materials synthesized from perlite by-product on retention of selected elements from soil pore water. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p.

- 482.(EUROCLAY 2019. International conference on clay science and technology).
- GII29 PÁLKOVÁ, Helena - BARLOG, Martin - PETRA, Lukáš - MADEJOVÁ, Jana - ŠIMON, Erik - ZIMOWSKA, Malgorzata. Influence of dry grinding on the structure of dioctahedral and trioctahedral smectites and organo-modified smectites. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 488.(EUROCLAY 2019. International conference on clay science and technology).
- GII30 RAKHMATULLIN, Aydar - MACHADO, Kelly - ZANGHI, Didier - POLOVOV, Ilya B. - ŠIMKO, František - BAKIROV, Rinat - MAKSIMTSEV, Konstantin V. - BESSADA, Catherine. Structural study by high temperature NMR and modeling Al-Sc alloy formation in NaF-ScF₃ melts. In MS11. 11th international symposium on molten salts - chemistry and technology, 19-23 Mai 2019, Orleans, France : program and abstracts. - France, 2019, p. 95.(MS11. International symposium on molten salts - chemistry and technology).
- GII31 SEDLÁČEK, Jaroslav - HNATKO, Miroslav - HIČÁK, Michal - LABUDOVÁ, Martina - GALUSKOVÁ, Dagmar - ŠAJGALÍK, Pavol. Bioactivity enhancement of silicon nitride ceramics by surface oxidation. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 387.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII32 SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - ŠKORŇA, Peter - MORENO RODRÍGUEZ, Daniel - TUNEGA, Daniel. Insight into the stability of beidellite intercalates. In BIT's 7th Annual Conference of AnalytiX-2019, April 12-14, 2019, Singapore : conference handbook.Exploring Innovative Advances and Applications. - Singapore, 2019, p. 78.(BIT's 7th Annual Conference of AnalytiX-2019).
- GII33 SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - ŠKORŇA, Peter - MORENO RODRÍGUEZ, Daniel - TUNEGA, Daniel. Tetraalkylphosphonium beidellite intercalates - structural stability by DFT method. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 556.(EUROCLAY 2019. International conference on clay science and technology).
- GII34 SLANÝ, Michal - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana. Effect of chain length and surfactant loading on the self-assembly of primary alkylammonium cations on montmorillonite. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 572.(EUROCLAY 2019. International conference on clay science and technology).
- GII35 ŠAJGALÍK, Pavol. Porous silicon nitride: A material for the bioactive composite implants. In ICACC 2019. 43rd International Conference & Exposition on Advanced Ceramics and Composites, January 27 - February 1, 2019, Daytona Beach, Florida, USA : abstract book. - USA : The American Ceramic Society, 2019, p. 199.(ICACC 2019. International Conference & Exposition on Advanced Ceramics and Composites).
- GII36 ŠAJGALÍK, Pavol - SEDLÁČEK, Jaroslav - KOVALČÍKOVÁ, Alexandra - HAN, X. - ZHANG, Chengyu. Ultra-high creep resistant silicon carbide ceramics. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 236.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII37 ŠAJGALÍK, Pavol. Ceramic research in Slovakia: potential for R&D cooperation. In CICC-11 : The Eleventh International Conference on High-Performance Ceramics, May 25-29, 2019, Kunming, China : abstract book. - China : The Chinese Ceramic Society, 2019, p. 386.(CICC-11 : International Conference on High-Performance Ceramics).
- GII38 ŠIMKO, František - RAKHMATULLIN, Aydar - VERON, Emmanuel - ALLIX, Mathieu - FLORIAN, Pierre - NETRIOVÁ, Zuzana - KORENKO, Michal - KAVEČANSKÝ, Viktor - BESSADA, Catherine. Oxo- and (oxo)(fluoro)-aluminates: Synthesis, stability and structure correlation. In MS11. 11th international symposium on molten salts - chemistry and technology, 19-23 Mai 2019, Orleans, France : program and abstracts. - France, 2019, p. 26.(MS11. International symposium on molten salts - chemistry and technology).
- GII39 ŠKORŇA, Peter - SCHOLTZOVÁ, Eva - JANKOVIČ, Ľuboš - TUNEGA, Daniel. Structural properties and spectroscopic characterization of choline-beidellite and acetylcholine-beidellite intercalates. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 571.(EUROCLAY 2019. International conference on clay science and technology).
- GII40 TALIMIAN, Ali - MICHÁLKOVÁ, Monika - GALUSEK, Dušan. Sintering of lithium hydroxide doped magnesium aluminate spinel. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 174.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII41 TATARKO, Peter - ZHOU, Xiaobing - GRASSO, Salvatore - DLOUHÝ, Ivo - REECE, Michael J. - FERRARIS, Monica. Electric current assisted solid-state diffusion joining of advanced SiC-based ceramics. In CICC-11 : The Eleventh International Conference on High-Performance Ceramics, May 25-29, 2019, Kunming, China : abstract book. - China : The Chinese Ceramic Society, 2019, p. 86.(CICC-11 : International Conference on High-Performance Ceramics).

- GII42 TATARKO, Peter - SAUNDERS, Theo G. - GRASSO, Salvatore - CHLUP, Zdeněk - DLOUHÝ, Ivo - REECE, Michael J. Interaction between SiC and Ti6Al4V in the SPS - From wetting studies to joining. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 177.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII43 TATARKOVÁ, Monika - HNATKO, Miroslav - SEDLÁČEK, Jaroslav - GALUSKOVÁ, Dagmar - KLEMENT, Róbert - ŠAJGALÍK, Pavol. Corrosion behaviour of silicon nitride and SiAlON in molten FLINAK. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 331.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII44 ÜNSAL, Hakan - SHEPA, Ivan - HANZEL, Ondrej - MÚDRA, Erika - VOJTKO, Marek - DUSZA, Ján - TATARKO, Peter. In situ synthesis and characterization of B4C-TiB2 fibers composites. In XVI ECerS Conference, Torino, Italy, 16-20 June 2019 : abstract book. - Italy, 2019, p. 701.(ECerS : Conference and Exhibition of the European Ceramic Society).
- GII45 ZIMOWSKA, Malgorzata - GURGUL, J. - SOCHA, Robert P. - PÁLKOVÁ, Helena - LATKA, K. - MATACHOWSKI, L. Laponite® derived porous heterostructures for hydrogen production. In EUROCLAY 2019. International conference on clay science and technology, 1st-5th July 2019, Sorbonne Université, Paris, France : book of abstracts. - Paris, France, 2019, p. 489.(EUROCLAY 2019. International conference on clay science and technology).

Ohlasy (citácie):

ABA Štúdie charakteru vedeckej monografie v časopisoch a zborníkoch vydané v zahraničných vydavateľstvách

- ABA01 BUJDÁK, Juraj. Hybrids with functional dyes : Chapter 18. In Inorganic nanosheets and nanosheet-based materials : Fundamentals and applications of two-dimensional systems. - Tokyo, Japan : Springer Japan, 2017, p. 419-465. ISBN 978-4-431-56494-2. ISSN 1571-5744.
- Citácie:
- [1.1] COIAI, Serena - JAVARONE, Stefano - CICOGNA, Francesca - OBERHAUSER, Werner - ONOR, Massimo - PUCCI, Andrea - MINEI, Pierpaolo - IASILLI, Giuseppe - PASSAGLIA, Elisa. Fluorescent LDPE and PLA nanocomposites containing fluorescein-modified layered double hydroxides and their ON/OFF responsive behavior towards humidity. In EUROPEAN POLYMER JOURNAL. ISSN 0014-3057, 2018, vol. 99, no., pp. 189-201., Registrované v: WOS
 - [1.1] KAWAMATA, Jun - SUZUKI, Yasutaka - TOMINAGA, Makoto. From adsorbed dyes to optical materials. In SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 361-375., Registrované v: WOS

ABC Kapitoly vo vedeckých monografiách vydané v zahraničných vydavateľstvách

- ABC01 KOMADEL, Peter - MADEJOVÁ, Jana. Acid activation of clay minerals. In Handbook of Clay Science. Vol. 1. - Elsevier, 2006, p. 263-287.
- Citácie:
- [1.1] AMARI, Abdelfattah - GANNOUNI, Hatem - KHAN, Mohammad I. - ALMESFER, Mohammed K. - ELKHALEEFA, Abubakr M. - GANNOUNI, Abdelaziz. Effect of Structure and Chemical Activation on the Adsorption Properties of Green Clay Minerals for the Removal of Cationic Dye. In APPLIED SCIENCES-BASEL. ISSN 2076-3417, 2018, vol. 8, no. 11, pp., Registrované v: WOS
 - [1.1] ANTONIO CECILIA, Juan - PARDO, Laura - POZO, Manuel - BELLIDO, Eva - FRANCO, Francisco. Microwave-Assisted Acid Activation of Clays Composed of 2:1 Clay Minerals: A Comparative Study. In MINERALS. ISSN 2075-163X, 2018, vol. 8, no. 9, pp., Registrované v: WOS
 - [1.1] AYAT, Moulkheir - BELBACHIR, Mohammed - RAHMOUNI, Abdelkader. Cationic polymerization of poly(alpha-methylstyrene-block-isobutyl vinyl ether) using Maghnite-H+ clay (Algerian MMT) as catalyst. In POLYMER BULLETIN. ISSN 0170-0839, 2018, vol. 75, no. 12, pp. 5355-5371., Registrované v: WOS
 - [1.1] CECILIA, J. A. - GARCIA-SANCHO, C. - VILARRASA-GARCIA, E. - JIMENEZ-JIMENEZ, J. - RODRIGUEZ-CASTELLON, E. Synthesis, Characterization, Uses and Applications of Porous Clays Heterostructures: A Review. In CHEMICAL RECORD. ISSN 1527-8999, 2018, vol. 18, no. 7-8, pp. 1085-1104., Registrované v: WOS
 - [1.1] CHARGUI, H. - HAJJAJI, W. - WOUTERS, J. - YANS, J. - JAMOSSI, F. Direct Orange 34 dye fixation by modified kaolin. In CLAY MINERALS. ISSN 0009-8558, 2018, vol. 53, no. 2, pp. 271-287., Registrované v: WOS
 - [1.1] DE ANDRADE, Julia R. - OLIVEIRA, Maria F. - DA SILVA, Meuris G. C. - VIEIRA, Melissa G. A. Adsorption of Pharmaceuticals from Water and Wastewater Using Nonconventional Low-Cost Materials: A Review. In INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH. ISSN 0888-5885, 2018, vol. 57, no. 9, pp. 3103-3127., Registrované v: WOS
 - [1.1] DJEBBAR, Mustapha - DJAFRI, Fatiha. ADSORPTION OF ZINC IONS IN WATER ON NATURAL AND TREATED CLAY. In CHEMISTRY & CHEMICAL TECHNOLOGY. ISSN 1996-4196, 2018, vol. 12, no. 2, pp. 272-278., Registrované v: WOS
 - [1.1] DOS SANTOS, E. C. - GATES, W. P. - MICHELS, L. - JURANYI, F. - MIKKELSEN, A. - DA SILVA, G. J. - FOSSUM, J. O. - BORDALLO, H. N. The pH influence on the intercalation of the bioactive agent ciprofloxacin in fluorohectorite. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 166, no., pp. 288-298., Registrované v: WOS
 - [1.1] GUO, Haijun - ZHANG, Hairong - CHEN, Xuefang - ZHANG, Liquan - HUANG, Chao - LI, Hailong - PENG, Fen -

HUANG, Yianlin - XIONG, Lian - OUYANG, Xinping - CHEN, Xinde - QIU, Xueqing. Catalytic upgrading of biopolyols derived from liquefaction of wheat straw over a high-performance and stable supported amorphous alloy catalyst. In *ENERGY CONVERSION AND MANAGEMENT*. ISSN 0196-8904, 2018, vol. 156, no., pp. 130-139., Registrované v: WOS

10. [1.1] KOOLI, Fethi - LIU, Yan - ABOUDI, Mostafa - RAKASS, Souad - HASSANI, Hicham Oudghiri - IBRAHIM, Sheikh Muhammad - AL-FAZE, Rawan. Removal Properties of Anionic Dye Eosin by Cetyltrimethylammonium Organo-Clays: The Effect of Counter-Ions and Regeneration Studies. In *MOLECULES*. ISSN 1420-3049, 2018, vol. 23, no. 9, pp., Registrované v: WOS

11. [1.1] LU, Yushen - DONG, Wenkai - WANG, Wenbo - DING, Junjie - WANG, Qin - HUI, Aiping - WANG, Aiqin. Optimal Synthesis of Environment-Friendly Iron Red Pigment from Natural Nanostructured Clay Minerals. In *NANOMATERIALS*. ISSN 2079-4991, 2018, vol. 8, no. 11, pp., Registrované v: WOS

12. [1.1] PARDO, Laura - ANTONIO CECILIA, Juan - LOPEZ-MORENO, Cristina - HERNANDEZ, Victor - POZO, Manuel - JOSE BENTABOL, Maria - FRANCO, Francisco. Influence of the Structure and Experimental Surface Modifications of 2:1 Clay Minerals on the Adsorption Properties of Methylene Blue. In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 8, pp., Registrované v: WOS

13. [1.1] RITZ, Michal - VALASKOVA, Marta. Infrared and Raman spectroscopy of three commercial vermiculites doped with cerium dioxide nanoparticles. In *SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY*. ISSN 1386-1425, 2018, vol. 201, no., pp. 39-45., Registrované v: WOS

14. [1.1] STAWINSKI, Wojciech - WEGRZYN, Agnieszka - MORDARSKI, Grzegorz - SKIBA, Michal - FREITAS, Olga - FIGUEIREDO, Sonia. Sustainable adsorbents formed from by-product of acid activation of vermiculite and leached-vermiculite-LDH hybrids for removal of industrial dyes and metal cations. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 161, no., pp. 6-14., Registrované v: WOS

15. [1.1] SUN, Bing - KHAN, Farooq-Ahmad - SUSS-FINK, Georg - THERRIEN, Bruno. Metal Catalysts Intercalated in Smectite Clays. In *ENCAPSULATED CATALYSTS*, 2017, vol., no., pp. 387-441., Registrované v: WOS

16. [1.1] TAVARES LUNA, Francisco Murilo - ANTONIO CECILIA, Juan - ALVES SABOYA, Rosana Maria - BARRERA, Deicy - SAPAG, Karim - RODRIGUEZ-CASTELLON, Enrique - CAVALCANTE, Celio Loureiro. Natural and Modified Montmorillonite Clays as Catalysts for Synthesis of Biolubricants. In *MATERIALS*. ISSN 1996-1944, 2018, vol. 11, no. 9, pp., Registrované v: WOS

17. [1.1] WEGRZYN, Agnieszka - STAWINSKI, Wojciech - FREITAS, Olga - KOMEDERA, Kamila - BLACHOWSKI, Artur - JECZMIONEK, Lukasz - DANKO, Tomasz - MORDARSKI, Grzegorz - FIGUEIREDO, Sonia. Study of adsorptive materials obtained by wet fine milling and acid activation of vermiculite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 155, no., pp. 37-49., Registrované v: WOS

18. [1.1] YAMAGUCHI, Tetsuo - OGAWA, Makoto. Photochromism of a Spiropyran in the Presence of a Synthetic Hectorite. In *CHEMISTRY LETTERS*. ISSN 0366-7022, 2018, vol. 47, no. 2, pp. 189-191., Registrované v: WOS

ABC02 KOMADEL, Peter - MADEJOVÁ, Jana. Acid activation of clay minerals. In *Handbook of Clay Science. A.Fundamentals*. 2nd. ed. - Oxford : Elsevier, 2013, p. 385-410. ISBN 978-0-08-098259-5. ISSN 1572-4352.

Citácie:

1. [1.2] ALEXANDER, J.A. - AHMAD ZAINI, M.A. - ABDULSALAM, S. - EL-NAFATY, U.A. - AROKE, U.O. Physicochemical characteristics of surface modified Dijah-Monkin bentonite. In *Particulate Science and Technology*, 2018, vol. 36, no. 3, pp. 286-297., Registrované v: SCOPUS

2. [1.2] ANJUM, H. - OBAID, M.A. - SHAMIM, M.Y. - MURUGESAN, T. Adsorption of benzene by "green" functionalization of montmorillonite. In *MATEC Web of Conferences*, 2018, vol. 150, art. no. 02001., Registrované v: SCOPUS

3. [1.2] JALIL, M.E.R. - BASCHINI, M. - SAPAG, K. Removal of ciprofloxacin from aqueous solutions using pillared clays. In *Materials*, 2017, vol. 10, no. 12, art. no. 1345., Registrované v: SCOPUS

4. [1.2] JALIL, M.E.R. - TOSCHI, F. - BASCHINI, M. - SAPAG, K. Silica pillared montmorillonites as possible adsorbents of antibiotics from water media. In *Applied Sciences (Switzerland)*, 2018, vol. 8, no. 8, art. no. 1403., Registrované v: SCOPUS

5. [1.2] MARSH, A. - HEATH, A. - PATUREAU, P. - EVERNDEN, M. - WALKER, P. Alkali activation behaviour of un-calcined montmorillonite and illite clay minerals. In *Applied Clay Science*, 2018, vol. 166, pp. 250-261., Registrované v: SCOPUS

ABC03 MADEJOVÁ, Jana - BALAN, Etienne - PETIT, Sabine. Application of vibrational spectroscopy to the characterization of phyllosilicates and other industrial minerals. In *Advances in the Characterization of Industrial Minerals*. - London : The Mineralogical Society of Great Britain and Ireland, 2011, p. 171-226. ISBN 978-0-903056-28-1.

Citácie:

1. [1.1] MAYDAGAN, Laura - FRANCHINI, Marta - IMPICCINI, Agnes - LENTZ, David - PATRIER, Patricia - BEAUFORT, Daniel. Chlorite, white mica and clay minerals as proximity indicators to ore in the shallow porphyry environment of Quebrada de la Mina deposit, Argentina. In *ORE GEOLOGY REVIEWS*. ISSN 0169-1368, 2018, vol. 92, no., pp. 297-317., Registrované v: WOS

2. [1.1] NDZANA, Georges Martial - HUANG, Li - WANG, Jin Bo - ZHANG, Zhi Yi. Characteristics of clay minerals in soil particles from an argillic horizon of Alfisol in central China. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 151, no., pp. 148-156., Registrované v: WOS

3. [1.1] PERETYAZHKO, T. S. - NILES, P. B. - SUTTER, B. - MORRIS, R. V. - AGRETI, D. G. - LE, L. - MING, D. W. Smectite formation in the presence of sulfuric acid: Implications for acidic smectite formation on early Mars. In *GEOCHIMICA ET COSMOCHIMICA ACTA*. ISSN 0016-7037, 2018, vol. 220, no., pp. 248-260., Registrované v: WOS

ABC04 MADEJOVÁ, Jana - PÁLKOVÁ, Helena - KOMADEL, Peter. IR spectroscopy of clay minerals and clay nanocomposites. In *Spectroscopic Properties of Inorganic and Organometallic Compounds : Techniques, materials and applications*. - Cambridge : UK, The Royal Society of Chemistry, 2010, 2010, vol. 41, p. 22-71.

Citácie:

1. [1.1] KHALFA, Aouda - MELLOUK, Senia - MAROUF-KHELIFA, Kheira - KHELIFA, Amine. Removal of catechol from water by modified dolomite: performance, spectroscopy, and mechanism. In *WATER SCIENCE AND TECHNOLOGY*. ISSN 0273-1223,

2018, vol. 77, no. 7, pp. 1920-1930., Registrované v: WOS

2. [1.1] MINK, Janos - MIHALY, Judith - NEMETH, Csaba - NEMETH, Peter - DREES, Markus - LOKSHIN, Boris V. - WOLF, Moritz - BUTLER, Ian S. - HAJBA, Laszlo. Preparation and characterization by infrared emission spectroscopy and applications of new mineral-based composite materials of biomedical interest. In *APPLIED SPECTROSCOPY REVIEWS*. ISSN 0570-4928, 2018, vol. 53, no. 6, pp. 439-485., Registrované v: WOS

3. [1.1] SILVA-VALENZUELA, Maria das Gracias - CHAMBI-PERALTA, Marvin Marco - SAYEG, Isaac Jamil - DE SOUZA CARVALHO, Flavio Machado - WANG, Shu Hui - VALENZUELA-DIAZ, Francisco Rolando. Enrichment of clay from Vitoria da Conquista (Brazil) for applications in cosmetics. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 155, no., pp. 111-119., Registrované v: WOS

4. [1.1] ZOPE, Indraneel Suhas. Decomposition Behavior of Metal-Ion Exchanged Clays. In *FIRE RETARDANCY BEHAVIOR OF POLYMER/CLAY NANOCOMPOSITES*. ISSN 2190-5053, 2018, vol., no., pp. 61-82., Registrované v: WOS

ABC05 MADEJOVÁ, Jana - GATES, W.P. - PETIT, Sabine. IR spectra of clay minerals : Chapter 5. In *Infrared and Raman spectroscopies of clay minerals*. - Netherlands : Elsevier, 2017, p. 107-149. ISBN 978-0-08-100355-8. ISSN 1572-4352.

Citácie:

1. [1.2] CUEVAS, Jaime - RUIZ, Ana Isabel - FERNÁNDEZ, Raúl - GONZÁLEZ-SANTAMARÍA, Daniel - ANGULO, María - ORTEGA, Almudena - TORRES, Elena - TURRERO, María Jesús. Authigenic clay minerals from interface reactions of concrete-clay engineered barriers: A new perspective on MG-clays formation in alkaline environments. In *Minerals*, 2018-09-01, 8, 9, pp., Registrované v: SCOPUS

2. [1.2] JELAVIĆ, S. - STIPP, S. L.S. - BOVET, N. Adsorption of organic ligands on low surface charge clay minerals: The composition in the aqueous interface region. In *Physical Chemistry Chemical Physics*. ISSN 14639076, 2018-01-01, 20, 25, pp. 17226-17233., Registrované v: SCOPUS

3. [1.2] MITSIS, I. - GODELITSAS, A. - GÖTTLICHER, J. - STEININGER, R. - GAMALETOS, P. N. - PERRAKI, M. - ABAD-ORTEGA, M. M. - STAMATAKIS, M. Chromium-bearing clays in altered ophiolitic rocks from Crommyonia (Soussaki) volcanic area, Attica, Greece. In *Applied Clay Science*. ISSN 01691317, 2018-09-15, 162, pp. 362-374., Registrované v: SCOPUS

4. [1.2] TORRES ASTORGA, Romina - DE LOS SANTOS VILLALOBOS, Sergio - VELASCO, Hugo - DOMÍNGUEZ-QUINTERO, Olioly - PEREIRA CARDOSO, Renan - MEIGIKOS DOS ANJOS, Roberto - DIAWARA, Yacouba - DERCON, Gerd - MABIT, Lionel. Exploring innovative techniques for identifying geochemical elements as fingerprints of sediment sources in an agricultural catchment of Argentina affected by soil erosion. In *Environmental Science and Pollution Research*. ISSN 09441344, 2018-07-01, 25, 21, pp. 20868-20879., Registrované v: SCOPUS

ABC06 MADEJOVÁ, Jana. Studies of reduced-charge smectites by near infrared spectroscopy. In *The Application of Vibrational Spectroscopy to Clay Minerals and Layered double Hydroxides*. Vol. 13. - Aurora CO, 2005, p. 169-202.

Citácie:

1. [1.2] CHRYSSIKOS, G. D. Modern Infrared and Raman Instrumentation and Sampling Methods. In *Developments in Clay Science*. ISSN 15724352, 2017-01-01, 8, pp. 34-63., Registrované v: SCOPUS

ABC07 MADEJOVÁ, Jana - KOMADEL, Peter. Information available from infrared spectra of the fine fractions of bentonites. In *The Application of Vibrational Spectroscopy to Clay Minerals and Layered double Hydroxides*. Vol. 13. - Aurora CO, 2005, p. 65-98.

Citácie:

1. [1.2] CHRYSSIKOS, G. D. Modern Infrared and Raman Instrumentation and Sampling Methods. In *Developments in Clay Science*. ISSN 15724352, 2017-01-01, 8, pp. 34-63., Registrované v: SCOPUS

2. [1.2] SHALDYBIN, M. V. - KRUPSKAYA, V. V. - GLOTOV, A. V. - DORJIEVA, O. V. - GONCHAROV, I. V. - SAMOILENKO, V. V. - DEEVA, E. S. - LOPUSHNYAK, Yu M. - BETHER, O. V. - ZAKUSIN, S. V. Petrography and clay mineralogy of anomaly luminescent layers in Bazhenov suite of Western Siberia sedimentary basin. In *Neftyanoe Khozyaystvo Oil Industry*. ISSN 00282448, 2018-02-01, 2, pp. 36-40., Registrované v: SCOPUS

ABC08 PETIT, Sabine - MADEJOVÁ, Jana. Fourier transform infrared spectroscopy. In *Handbook of Clay Science. B. Techniques and Applications*. Second edition. - Oxford : Elsevier, 2013, p. 213-232. ISBN 978-0-08-098258-8. ISSN 1572-4352.

Citácie:

1. [1.2] KASPRZHITSKII, Anton - LAZORENKO, Georgy - KHATER, Antoine - YAVNA, Victor. Mid-infrared spectroscopic assessment of plasticity characteristics of clay soils. In *Minerals*, 2018-05-01, 8, 5, pp., Registrované v: SCOPUS

2. [1.2] SCHNETZER, Florian - JOHNSTON, Cliff T. - PREMACHANDRA, Gnanasiri S. - GIRAUDO, Nicolas - SCHUHMANN, Rainer - THISEN, Peter - EMMERICH, Katja. Impact of Intrinsic Structural Properties on the Hydration of 2:1 Layer Silicates. In *ACS Earth and Space Chemistry*, 2017-12-21, 1, 10, pp. 608-620., Registrované v: SCOPUS

3. [2.2] LAZORENKO, Georgy - KASPRZHITSKII, Anton - YAVNA, Victor. Synthesis and structural characterization of betaine- and imidazoline-based organoclays. In *Chemical Physics Letters*. ISSN 00092614, 2018-01-16, 692, pp. 264-270., Registrované v: SCOPUS

*ADC Vedecké práce v zahraničných karentovaných časopisoch

ADC01 KOŮŠ, Miroslav - STEINER, Bohumil - MIČOVÁ, Júlia - LANGER, Vratislav - ĐURÍK, M. - GYEPESOVÁ, Dalma. Synthesis and structure determination of some sugar amino acids related to alanine and 6-deoxymannojirimycin. In *Carbohydrate Research*, 2001, vol. 332, p. 351-361. (2000: 1.606 - IF, karentované - CCC). (2001 - Current Contents). ISSN 0008-6215.

Citácie:

1. [1.1] GRYGORENKO, Oleksandr O. - BIITSEVA, Angelina V. - ZHERSH, Serhii. Amino sulfonic acids, peptidosulfonamides

and other related compounds. In *TETRAHEDRON*. ISSN 0040-4020, 2018, vol. 74, no. 13, pp. 1355-1421., Registrované v: WOS
 ADC02 MIČOVÁ, Júlia - STEINER, Bohumil - KOŇŠ, Miroslav - LANGER, Vratislav - ĐURÍK, M. - GYEPESOVÁ, Dalma - SMRČOK, Ľubomír. Some amino sugars structurally related to 6-deoxymannojirimycin precursors prepared from methyl 6-deoxy-2,3-O-isopropylidene- α -D-lyxo-hexofuranosid-5-ulose and methyl 2,3-O-isopropylidene- β -D-lyxo-pentodialdo-1,4-furanoside. In *Carbohydrate Research*, 2002, vol. 337, no. 8, p. 663-672. (2001: 1.349 - IF, karentované - CCC). (2002 - Current Contents). ISSN 0008-6215.

Citácie:

1. [1.1] MISTRY, Priyank P. - DESAI, Vikash A. *SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL EVOLUTION OF VARIOUS NOVEL HETEROCYCLIC COMPOUNDS OF HYDANTOIN AND PIPERAZINE*. In *HETEROCYCLIC LETTERS*. ISSN 2231-3087, 2018, vol. 8, no. 1, pp. 145-154., Registrované v: WOS

ADC03 SVRČEK, M. - BAŇACKÝ, P. - BISKUPIČ, S. - PELIKÁN, P. - ZAJAC, A. - NOGA, Jozef. Adiabatic correction to the energy of molecular systems: the CPHF equivalent of the Born-Handy formula. In *Chemical Physics Letters*, 1999, vol. 299, p. 151-157. (1998: 2.260 - IF, karentované - CCC). (1999 - Current Contents).

Citácie:

1. [1.1] SHAMASUNDAR, K. R. *Diagonal Born-Oppenheimer correction for coupled-cluster wave-functions*. In *MOLECULAR PHYSICS*. ISSN 0026-8976, 2018, vol. 116, no. 11, pp. 1483-1495., Registrované v: WOS

ADCA Vedecké práce v zahraničných karentovaných časopisoch – impaktovaných

ADCA01 ALDERMAN, Oliver - LIŠKA, Marek - MACHÁČEK, Jan - BENMORE, C.J. - LIN, A. - TAMALONIS, A. - WEBER, J.K.R. Temperature-driven structural transitions in molten sodium borates Na₂O-B₂O₃: X-ray diffraction, thermodynamic modeling, and implications for topological constraint theory. In *Journal of Physical Chemistry C*, 2016, vol. 120, no. 1, p. 553-560. (2015: 4.509 - IF, Q1 - JCR, 1.917 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 1932-7447.

Citácie:

1. [1.1] OHKUBO, Takahiro - TSUCHIDA, Eiji - DEGUCHI, Kenzo - OHKI, Shinobu - SHIMIZU, Tadashi - OTOMO, Toshiya - IWADATE, Yasuhiko. *Insights from abinitio molecular dynamics simulations for a multicomponent oxide glass*. In *JOURNAL OF THE AMERICAN CERAMIC SOCIETY*. ISSN 0002-7820, 2018, vol. 101, no. 3, pp. 1122-1134., Registrované v: WOS

ADCA02 ANDREJKOVIČOVÁ, Slávka - JANOTKA, Ivan - KOMADEL, Peter. Evaluation of geotechnical properties of bentonite from Lieskovec deposit, Slovakia. In *Applied Clay Science*, 2008, vol. 38, no. 3-4, p. 297-303. (2007: 1.861 - IF). ISSN 0169-1317.

Citácie:

1. [1.1] CHEN, S. J. - WANG, S. W. - LI, L. L. - QU, J. Z. - TAO, X. X. - HE, H. *Exploration on the mechanism of enhancing low-rank coal flotation with cationic surfactant in the presence of oily collector*. In *FUEL*. ISSN 0016-2361, 2018, vol. 227, p. 190-198., Registrované v: WOS

ADCA03 ARBUZNIKOV, Alexei V. - KAUPP, Martin - MALKIN, Vladimír - REVIKINE, Roman - MALKINA, Olga. Validation study of meta-GGA functionals and of a model exchange-correlation potential in density functional calculations of EPR parameters. In *Physical Chemistry Chemical Physics*, 2002, vol. 4, no. 22, p. 5467-5474.

Citácie:

1. [1.1] SINGH, Saurabh Kumar - ATANASOV, Mihail - NEESE, Frank. *Challenges in Multireference Perturbation Theory for the Calculations of the g-Tensor of First-Row Transition-Metal Complexes*. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 9, pp. 4662-4677., Registrované v: WOS

ADCA04 AZZI, Andreza de Almeida - OSACKÝ, Marek - UHLÍK, Peter - ČAPLOVIČOVÁ, Mária - ZANARDO, Antenor - MADEJOVÁ, Jana. Characterization of clays from the Corumbataí formation used as raw material for ceramic industry in the Santa Gertrudes district, Sao Paulo, Brazil. In *Applied Clay Science*, 2016, vol. 132-133, p. 232-242. (2015: 2.586 - IF, Q1 - JCR, 0.808 - SJR, Q2 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] AGHAYEV, Tural - KUCUKUYSAL, Ceren. *Ceramic properties of Usak clay in comparison with Ukrainian clay*. In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 4, pp. 549-562., Registrované v: WOS

2. [1.1] NDZANA, Georges Martial - HUANG, Li - WANG, Jin Bo - ZHANG, Zhi Yi. *Characteristics of clay minerals in soil particles from an argillite horizon of Alfisol in central China*. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 151, no., pp. 148-156., Registrované v: WOS

ADCA05 BAČA, Ľuboš - LENČEŠ, Zoltán - JOGL, Christian - NEUBAUER, Erich - VITKOVIČ, Martin - MERSTALLINGER, Andreas - ŠAJGALÍK, Pavol. Microstructure evolution and tribological properties of TiB₂/Ni-Ta cermets. In *Journal of the European Ceramic Society*, 2012, vol. 32, no. 9, p. 1941-1948. (2011: 2.353 - IF, 1.343 - SJR, karentované - CCC). (2012 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] YIN, Zengbin - YUAN, Juntang - XU, Weiwei - CHEN, Mingdan - YAN, Shiyu - WANG, Zhenhua. *Effect of Ni and graphene on microstructure and toughness of titanium boride ceramic tool material prepared by spark plasma sintering*. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 16, pp. 20299-20305., Registrované v: WOS

- ADCA06 BAČA, Ľuboš - LENČEŠ, Zoltán - STELZER, Nils. Phase, microstructure evolution and sintering of Sr-doped TiB₂ precursors. In Journal of the European Ceramic Society, 2011, vol. 31, no. 8, p. 1465-1471. (2010: 2.574 - IF, karentované - CCC). (2011 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] LIN, Jia - YANG, Yihang - ZHANG, Houan - LIN, Qin - ZHU, Bin. Synthesis and characterization of in-situ CNTs reinforced TiB₂-based composite by CVD using Ni catalysts. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 2, pp. 2042-2047., Registrované v: WOS

- ADCA07 BALÁZSI, Csaba - FOGARASSY, Zsolt - TAPASZTÓ, Orsolya - KAILER, Andreas - SCHRÖDER, Christian - PARCHOVIANSKÝ, Milan - GALUSEK, Dušan - DUSZA, Ján - BALAZSI, K. Si₃N₄/graphene nanocomposites for tribological application in aqueous environments prepared by attritor milling and hot pressing. In Journal of the European Ceramic Society, 2017, vol. 37, p. 3797-3804. (2016: 3.454 - IF, Q1 - JCR, 1.142 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0955-2219.

Citácie:

1. [1.1] CHICINAS, H. F. - JUCAN, D. O. - MARINCA, T. F. - NEAMTU, B. - CONTIU, G. - GOETZE, P. - ECKERT, A. - POPA, Co. Influence of milling media on the structure and agglomeration behaviour of some hardmetal powder. In POWDER METALLURGY. ISSN 0032-5899, 2018, vol. 61, no. 4, pp. 342-347., Registrované v: WOS

2. [1.1] CINAR, Alper - BASKUT, Sinem - SEYHAN, A. Tugrul - TURAN, Servet. Tailoring the properties of spark plasma sintered SiAlON containing graphene nanoplatelets by using different exfoliation and size reduction techniques: Anisotropic mechanical and thermal properties. In JOURNAL OF THE EUROPEAN CERAMIC SOCIETY. ISSN 0955-2219, 2018, vol. 38, no. 4, pp. 1299-1310., Registrované v: WOS

3. [1.1] LIU, Jiongjie - WANG, Zixi - YIN, Bing - YANG, Jun - SUN, Qichun - LIU, Yulin - TAN, Hui - QIAO, Zhuhui. A novel method to prepare self-lubricity of Si₃N₄/Ag composite: Microstructure, mechanical and tribological properties. In JOURNAL OF THE AMERICAN CERAMIC SOCIETY. ISSN 0002-7820, 2018, vol. 101, no. 9, pp. 3745-3748., Registrované v: WOS

4. [1.1] LIU, Jiongjie - YANG, Jun - YU, Yuan - SUN, Qichun - QIAO, Zhuhui - LIU, Weimin. Self-Lubricating Si₃N₄-based composites toughened by in situ formation of silver. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 12, pp. 14327-14334., Registrované v: WOS

5. [1.1] LLORENTE, Javier - BELMONTE, Manuel. Friction and wear behaviour of silicon carbide/graphene composites under isooctane lubrication. In JOURNAL OF THE EUROPEAN CERAMIC SOCIETY. ISSN 0955-2219, 2018, vol. 38, no. 10, pp. 3441-3446., Registrované v: WOS

6. [1.1] WU, Lupeng - XIE, Zhijie - GU, Le - SONG, Baoyu - WANG, Liqin. Investigation of the tribological behavior of graphene oxide nanoplates as lubricant additives for ceramic/steel contact. In TRIBOLOGY INTERNATIONAL. ISSN 0301-679X, 2018, vol. 128, no., pp. 113-120., Registrované v: WOS

- ADCA08 BALOG, Miroslav - ŠAJGALÍK, Pavol - HNATKO, Miroslav - LENČEŠ, Zoltán - MONTEVERDE, E. - KEČKÉŠ, Jozef - HUANG, J.-L. Nano- versus macro-hardness of liquid phase sintered SiC. In Journal of the European Ceramic Society, 2005, vol. 25, no. 4, p. 529-534. ISSN 0955-2219.

Citácie:

1. [1.1] MALIK, Rohit - KIM, Hyun-Min - KIM, Young-Wook - KIM, Kwang Joo. Grain-growth-induced high electrical conductivity in SiC-BN composites. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 14, pp. 16394-16399., Registrované v: WOS

2. [1.1] SABU, Ummen - MAJUMDAR, Bhaskar - SAHA, Bhaskar P. - DAS, Dibakar. Spark Plasma Sintering of Silicon Carbide with Al₂O₃ and CaO: Densification Behavior, Phase Evolution and Mechanical Properties. In TRANSACTIONS OF THE INDIAN CERAMIC SOCIETY. ISSN 0371-750X, 2018, vol. 77, no. 4, pp. 202-208., Registrované v: WOS

- ADCA09 BALTRUSAITIS, Jonas - BUČKO, Tomáš - MICHAELS, W. - MAKKEE, M. - MUL, G. Catalytic methyl mercaptan coupling to ethylene in chabazite: DFT study of the first C-C bond formation. In Applied Catalysis B: Environmental, 2016, vol. 187, p. 195-203. (2015: 8.328 - IF, Q1 - JCR, 2.326 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0926-3373.

Citácie:

1. [1.1] LI, Qing-Ming - ZHANG, Min - WANG, Chuan-Ming - ZHU, Yi-An - ZHOU, Xing-Gui - XIE, Zai-Ku. Effects of methylating agent and Bronsted acidity on methylation activity of olefins in CHA-structured zeolites: A periodic DFT study. In MOLECULAR CATALYSIS. ISSN 2468-8231, 2018, vol. 446, no., pp. 106-114., Registrované v: WOS

- ADCA10 BAŇACKÝ, P. - NOGA, Jozef - SZŐCS, Vojtech. Electronic structure of single-wall silicon nanotubes and silicon nanoribbons: helical symmetry treatment and effect of dimensionality. In Advances in Condensed Matter Physics, 2013, vol. 2013, article ID 374371, 16 p. (2012: 1.175 - IF, 0.710 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 1687-8108.

Citácie:

1. [1.1] HOWLADER, Ashraful Hossain - ISLAM, Md Sherajul - ISLAM, A. S. M. Jannatul. A Study on Phonon Transmission of (10,0) Silicon Nanotube with Atomic Vacancies. In 2018 21ST INTERNATIONAL CONFERENCE OF COMPUTER AND INFORMATION TECHNOLOGY (ICCIT). ISSN 2474-9648, 2018, vol., no., pp., Registrované v: WOS

- ADCA11 BARAN, Peter - BOČA, Miroslav - BOČA, Roman - KRUTOŠÍKOVÁ, Alžbeta - MIKLOVIČ, Jozef - PELIKÁN, Juraj - TITIŠ, Ján. Structural characterization, spectral and magnetic properties of isothiocyanate nickel(II) complexes with furopyridine derivatives. In Polyhedron, 2005, vol. 24, no. 12, p. 1510-1516.

Citácie:

1. [1.1] CERNAK, Juraj - HEGEDUS, Michal - VAHOVSKA, Lucia - KUCHAR, Juraj - SOLTESOVA, Daniela - CIZMAR, Erik - FEHER, Alexander - FALVELLO, L. R. Syntheses, crystal structures and magnetic properties of complexes based on [Ni(L-

- L(3)](2+) complex cations with dimethyl derivatives of 2,2'-bipyridine and TCNQ. In *SOLID STATE SCIENCES*. ISSN 1293-2558, 2018, vol. 77, no., pp. 27-36., Registrované v: WOS
2. [1.1] CERNAK, Juraj - KOCANOVA, Ivana - KUCHAR, Juraj - HILLARD, Elizabeth A. - CLERAC, Rodolphe. Formation of the unprecedented trinuclear $[\text{NiCu}_2(\text{CN})_8](4-)$ complex anion within the crystal structure of $[\text{Ni}(5,5'\text{-dmbpy})(3)](2)[\text{NiCu}_2(\text{CN})_8]\text{center dot } 6\text{H}_2\text{O}$. In *INORGANIC CHEMISTRY COMMUNICATIONS*. ISSN 1387-7003, 2018, vol. 91, no., pp. 16-19., Registrované v: WOS
3. [1.1] LOPEZ LAGO, Elena - SEIJAS, Julio A. - DE PEDRO, Imanol - RODRIGUEZ FERNANDEZ, Jesus - PILAR VAZQUEZ-TATO, M. - ANTONIO GONZALEZ, Jesus - RILO, Esther - SEGADÉ, Luisa - CABEZA, Oscar - RODRIGUEZ FERNANDEZ, Carlos Damian - AROSA, Yago - ALGNAMAT, Bilal S. - VARELA, Luis M. - TRONCOSO, Jacobo - DE LA FUENTE, Raul. Structural and physical properties of a new reversible and continuous thermochromic ionic liquid in a wide temperature interval: $[\text{BMIM}](4)[\text{Ni}(\text{NCS})(6)]$. In *NEW JOURNAL OF CHEMISTRY*. ISSN 1144-0546, 2018, vol. 42, no. 19, pp. 15561-15571., Registrované v: WOS
4. [1.1] SAGIR, Hozeyfa - YADAV, Vijay B. - SHAMIM, Shayna - KUMAR, Akhilesh - YADAV, Neetu - ANSARI, Mohd Danish - SIDDIQUI, I. R. An Eco-Compatible synthesis of Substituted Hexahydro-Furo[3,2-c]pyridine Analogues with the Chitosan/Ionic Liquid Coupled Catalytic System. In *CHEMISTRYSELECT*. ISSN 2365-6549, 2018, vol. 3, no. 38, pp. 10799-10804., Registrované v: WOS

ADCA12 BARTLETT, Rodney J. - KUCHARSKI, Stanislaw A. - NOGA, Jozef. Alternative coupled-cluster ansätze II. The unitary coupled-cluster method. In *Chemical Physics Letters*, 1989, vol. 155, no. 1, p. 133-140.

Citácie:

1. [1.1] BARKOUTSOS, Panagiotis Kl - GONTHIER, Jerome F. - SOKOLOV, Igor - MOLL, Nikolaj - SALIS, Gian - FUHRER, Andreas - GANZHORN, Marc - EGGER, Daniel J. - TROYER, Matthias - MEZZACAPPO, Antonio - FILIPP, Stefan - TAVERNELLI, Ivano. Quantum algorithms for electronic structure calculations: Particle-hole Hamiltonian and optimized wave-function expansions. In *PHYSICAL REVIEW A*. ISSN 2469-9926, 2018, vol. 98, no. 2, pp., Registrované v: WOS
2. [1.1] COPAN, Andreas V. - SOKOLOV, Alexander Yu. Linear-Response Density Cumulant Theory for Excited Electronic States. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 8, pp. 4097-4108., Registrované v: WOS
3. [1.1] HARSHA, Gaurav - SHIOZAKI, Toru - SCUSERIA, Gustavo E. On the difference between variational and unitary coupled cluster theories. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 4, pp., Registrované v: WOS
4. [1.1] HEMPEL, Cornelius - MAIER, Christine - ROMERO, Jonathan - MCCLEAN, Jarrod - MONZ, Thomas - SHEN, Heng - JURCEVIC, Petar - LANYON, Ben P. - LOVE, Peter - BABBUSH, Ryan - ASPURU-GUZZIK, Alan - BLATT, Rainer - ROOS, Christian F. Quantum Chemistry Calculations on a Trapped-Ion Quantum Simulator. In *PHYSICAL REVIEW X*. ISSN 2160-3308, 2018, vol. 8, no. 3, pp., Registrované v: WOS
5. [1.1] KOWALSKI, Karol. Properties of coupled-cluster equations originating in excitation sub-algebras. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 9, pp., Registrované v: WOS
6. [1.1] LIU, Junzi - ASTHANA, Ayush - CHENG, Lan - MUKHERJEE, Debashis. Unitary coupled-cluster based self-consistent polarization propagator theory: A third-order formulation and pilot applications. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 24, pp., Registrované v: WOS
7. [1.1] SOKOLOV, Alexander Yu. Multi-reference algebraic diagrammatic construction theory for excited states: General formulation and first-order implementation. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 20, pp., Registrované v: WOS
8. [1.1] TALUKDAR, Kaushik - SASMAL, Sudip - NAYAK, Malaya K. - VAVAL, Nayana - PAL, Sourav. Correlation trends in the magnetic hyperfine structure of atoms: A relativistic coupled-cluster case study. In *PHYSICAL REVIEW A*. ISSN 2469-9926, 2018, vol. 98, no. 2, pp., Registrované v: WOS

ADCA13 BARTLETT, Rodney J. - NOGA, Jozef. The expectation value coupled-cluster method and analytical energy derivatives. In *Chemical Physics Letters*, 1988, vol. 150, no. 1-2, p. 29-36.

Citácie:

1. [1.1] TALUKDAR, Kaushik - SASMAL, Sudip - NAYAK, Malaya K. - VAVAL, Nayana - PAL, Sourav. Correlation trends in the magnetic hyperfine structure of atoms: A relativistic coupled-cluster case study. In *PHYSICAL REVIEW A*. ISSN 2469-9926, 2018, vol. 98, no. 2, pp., Registrované v: WOS

ADCA14 BARTLETT, Rodney J. - WATTS, J. D. - KUCHARSKI, Stanislaw A. - NOGA, Jozef. Non-iterative fifth-order triple and quadruple excitation energy corrections in correlated methods. In *Chemical Physics Letters*, 1990, vol. 165, no. 6, p. 513-522.

Citácie:

1. [1.1] ABBOTT, Adam S. - GLICK, Zach L. - SCHAEFER, Henry F. Reinterpretation of the electronic absorption spectrum of the methylene amidogen radical (H_2CN). In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 9, pp., Registrované v: WOS
2. [1.1] ABDO, Yasmeen A. - WEEKS, Justin W. - LAYFIELD, William - TREMLETT, William M. - GRAHAM, Joshua W. - TABOR, Mikayla E. - CAUSEY, Sarah E. - CARR, Jeremy M. - TSCHUMPER, Gregory S. Intramolecular Hydrogen Bonding in α -Epoxy Alcohols: A Conformational Analysis of 1,2-Dialkyl-2,3-epoxycyclopentanol Diastereomers. In *CHEMISTRY LETTERS*. ISSN 0366-7022, 2018, vol. 47, no. 2, pp. 156-159., Registrované v: WOS
3. [1.1] ARMENTROUT, P. B. - COX, Richard M. - SWEENEY, Brendan C. - ARD, Shaun G. - SHUMAN, Nicholas S. - VIGGIANO, Albert A. Lanthanides as Catalysts: Guided Ion Beam and Theoretical Studies of $\text{Sm}^+ + \text{COS}$. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 3, pp. 737-749., Registrované v: WOS
4. [1.1] DEMIREVA, Maria - ARMENTROUT, P. B. Activation of CO_2 by Gadolinium Cation (Gd^+): Energetics and Mechanism from Experiment and Theory. In *TOPICS IN CATALYSIS*. ISSN 1022-5528, 2018, vol. 61, no. 1-2, pp. 3-19., Registrované v: WOS
5. [1.1] DEMIREVA, Maria - ARMENTROUT, P. B. Activation of H_2 by Gadolinium Cation (Gd^+): Bond Energy of GdH^+ and Mechanistic Insights from Guided Ion Beam and Theoretical Studies. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 3, pp. 750-761., Registrované v: WOS

6. [1.1] DEMIREVA, Maria - ARMENTROUT, P. B. Samarium cation (Sm^{+}) reactions with H-2, D-2, and HD: SmH^{+} bond energy and mechanistic insights from guided ion beam and theoretical studies. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 16, pp., Registrované v: WOS
7. [1.1] ECKHARDT, Andre K. - GERBIG, Dennis - SCHREINER, Peter R. Heavy Atom Secondary Kinetic Isotope Effect on H-Tunneling. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 5, pp. 1488-1495., Registrované v: WOS
8. [1.1] IVANIC, Joseph - SCHMIDT, Michael W. Hybrid Correlation Energy (HyCE): An Approach Based on Separate Evaluations of Internal and External Components. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 23, pp. 5223-5237., Registrované v: WOS
9. [1.1] JAGAU, Thomas-C. Coupled-cluster treatment of molecular strong-field ionization. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 20, pp., Registrované v: WOS
10. [1.1] JAGAU, Thomas-C. Non-iterative triple excitations in equation-of-motion coupled-cluster theory for electron attachment with applications to bound and temporary anions. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 2, pp., Registrované v: WOS
11. [1.1] KAPLAN, Ilya G. - MIRANDA, Ulises - TRAKHTENBERG, Leonid I. Study of the In_2O_3 molecule in the free state and in the crystal. In *MOLECULAR PHYSICS*. ISSN 0026-8976, 2018, vol. 116, no. 5-6, pp. 678-685., Registrované v: WOS
12. [1.1] KARTON, Amir - MCKEMMISH, Laura K. Can Popular DFT Approximations and Truncated Coupled Cluster Theory Describe the Potential Energy Surface of the Beryllium Dimer? In *AUSTRALIAN JOURNAL OF CHEMISTRY*. ISSN 0004-9425, 2018, vol. 71, no. 10, pp. 804-810., Registrované v: WOS
13. [1.1] KIM, Jeongnim - BACZEWSKI, Andrew T. - BEAUDET, Todd D. - BENALI, Anouar - BENNETT, M. Chandler - BERRILL, Mark A. - BLUNT, Nick S. - JOSUE, Edgar - BORDA, Landinez - CASULA, Michele - et al. QMCPACK: an open source ab initio quantum Monte Carlo package for the electronic structure of atoms, molecules and solids. In *JOURNAL OF PHYSICS-CONDENSED MATTER*. ISSN 0953-8984, 2018, vol. 30, no. 19, pp., Registrované v: WOS
14. [1.1] LI, Wan-Lu - LU, Jun-Bo - ZHAO, Lili - PONEC, Robert - COOPER, David L. - LI, Jun - FRENKING, Gernot. Electronic Structure and Bonding Situation in M_2O_2 ($\text{M} = \text{Be}, \text{Mg}, \text{Ca}$) Rhombic Clusters. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 10, pp. 2816-2822., Registrované v: WOS
15. [1.1] MISIEWICZ, Jonathon P. - ELLIOTT, Sarah N. - MOORE, Kevin B. - SCHAEFER, Henry F. Re-examining ammonia addition to the Criegee intermediate: converging to chemical accuracy. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 11, pp. 7479-7491., Registrované v: WOS
16. [1.1] SAFAEI, Zahra - SHIROUDI, Abolfazl - PADASH, Rahman - SILLANPAA, Mika - ZAHEDI, Ehsan. Reaction mechanisms and kinetics of the beta-elimination processes of compounds $\text{CHF}_2\text{CH}_2\text{SiFnMe}_{3-n}$ ($n=0-3$): DFT and CBS-QB3 methods using Rice-Ramsperger-Kassel-Marcus and transition state theories. In *JOURNAL OF FLUORINE CHEMISTRY*. ISSN 0022-1139, 2018, vol. 216, no., pp. 71-80., Registrované v: WOS
17. [1.1] SHAHI, Abhishek - MCCASLIN, Laura - ALBECK, Yishai - CONTINETTI, Robert E. - GERBER, R. Benny - STRASSER, Daniel. Double Photodetachment of F-center dot H_2O : Experimental and Theoretical Studies of $[\text{F center dot H}_2\text{O}](+)$. In *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*. ISSN 1948-7185, 2018, vol. 9, no. 23, pp. 6808-6813., Registrované v: WOS
18. [1.1] SUN, Zhi - MOORE, Kevin B. - HILL, J. Grant - PETERSON, Kirk A. - SCHAEFER, Henry F. - HOFFMANN, Roald. Alkali-Metal Trihalides: MX_3 - Ion Pair or MX_2 -X-2 Complex? In *JOURNAL OF PHYSICAL CHEMISTRY B*. ISSN 1520-6106, 2018, vol. 122, no. 13, pp. 3339-3353., Registrované v: WOS
19. [1.1] THANH LAM NGUYEN - STANTON, John F. Three-Dimensional Master Equation (3DME) Approach. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 38, pp. 7757-7767., Registrované v: WOS
20. [1.1] THANH LAM NGUYEN - THORPE, James H. - BROSS, David H. - RUSCIC, Branko - STANTON, John F. Unimolecular Reaction of Methyl Isocyanide to Acetonitrile: A High-Level Theoretical Study. In *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*. ISSN 1948-7185, 2018, vol. 9, no. 10, pp. 2532-2538., Registrované v: WOS
21. [1.1] THIMMAKONDU, Venkatesan S. - KARTON, Amir. The quest for the carbene bent-pentadienyldiene isomer of C_5H_2 . In *CHEMICAL PHYSICS*. ISSN 0301-0104, 2018, vol. 515, no., pp. 411-417., Registrované v: WOS
22. [1.1] THIRUMOORTHY, Krishnan - KARTON, Amir - THIMMAKONDU, Venkatesan S. From High-Energy C_7H_2 Isomers with A Planar Tetracoordinate Carbon Atom to An Experimentally Known Carbene. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 46, pp. 9054-9064., Registrované v: WOS
23. [1.1] THOMAS, Daniel A. - MARIANSKI, Mateusz - MUCHA, Eike - MEIJER, Gerard - JOHNSON, Mark A. - VON HELDEN, Gert. Ground-State Structure of the Proton-Bound Formate Dimer by Cold-Ion Infrared Action Spectroscopy. In *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*. ISSN 1433-7851, 2018, vol. 57, no. 33, pp. 10615-10619., Registrované v: WOS
24. [1.1] THOMAS, Daniel A. - MUCHA, Eike - GEWINNER, Sandy - SCHOELLKOPF, Wieland - MEIJER, Gerard - VON HELDEN, Gert. Vibrational Spectroscopy of Fluoroformate, FCO_2^- , Trapped in Helium Nanodroplets. In *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*. ISSN 1948-7185, 2018, vol. 9, no. 9, pp. 2305-2310., Registrované v: WOS
25. [1.1] ULLAH, Saif - DENIS, Pablo A. - SATO, Fernando. Coupled cluster and density functional investigation of the neutral sodium-benzene and potassium-benzene complexes. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 706, no., pp. 343-347., Registrované v: WOS
26. [1.1] UNAL, Asli - BOZKAYA, Ugur. Anionic water pentamer and hexamer clusters: An extensive study of structures and energetics. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 12, pp., Registrované v: WOS
27. [1.1] WAGNER, J. Philipp - MCDONALD, David C. - DUNCAN, Michael A. An Argon-Oxygen Covalent Bond in the ArOH^+ Molecular Ion. In *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*. ISSN 1433-7851, 2018, vol. 57, no. 18, pp. 5081-5085., Registrované v: WOS
28. [1.1] WELBORN, Matthew - MANBY, Frederick R. - MILLER, Thomas F. Even-handed subsystem selection in projection-based embedding. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 14, pp., Registrované v: WOS
29. [1.1] WIENS, Avery E. - COPAN, Andreas V. - ROSSOMME, Elliot C. - AROEIRA, Gustavo J. R. - BERNSTEIN, Olivia M. - AGARWAL, Jay - SCHAEFER, Henry F. Reinterpreting the infrared spectrum of H plus HCN: Methylene amidogen radical and its coproducts. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 1, pp., Registrované v: WOS

Resonance energy transfer between dye molecules in colloids of a layered silicate. The effect of dye surface concentration. In *Journal of Physical Chemistry C*, 2017, vol. 121, p. 8300-8309. (2016: 4.536 - IF, Q1 - JCR, 1.964 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 1932-7447.

Citácie:

1. [1.1] HAO, Jiaojiao - YANG, Yang. The effects of different heterocycles and solvents on the ESIPT mechanisms of three novel photoactive mono-formylated benzoxazole derivatives. In *ORGANIC CHEMISTRY FRONTIERS*. ISSN 2052-4129, 2018, vol. 5, no. 14, pp. 2234-2243., Registrované v: WOS
2. [1.1] KAWAMATA, Jun - SUZUKI, Yasutaka - TOMINAGA, Makoto. From adsorbed dyes to optical materials. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9*. ISSN 1572-4352, 2018, vol. 9, no., pp. 361-375., Registrované v: WOS
3. [1.1] SANO, Keito - SONOTANI, Amane - TATSUMI, Daichi - OHTANI, Yuta - SHIMADA, Tetsuya - TAKAGI, Shinsuke. Characterization of dispersed titania nanosheet under aqueous conditions and its complex formation behavior with cationic porphyrin. In *JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY*. ISSN 1010-6030, 2018, vol. 353, no., pp. 597-601., Registrované v: WOS

ADCA16 BELUŠÁKOVÁ, Silvia - LANG, Kamil - BUJDÁK, Juraj. Hybrid systems based on layered silicate and organic dyes for cascade energy transfer. In *Journal of Physical Chemistry C*, 2015, vol. 119, no. 38, p. 21784-21794. (2014: 4.772 - IF, Q1 - JCR, 2.027 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 1932-7447.

Citácie:

1. [1.1] LI, Xiaochuan - HAN, Yujie - MIN, Kyeongsu - SON, Young-A. Configuration of white light emission by coumarin and naphthalimide. In *MOLECULAR CRYSTALS AND LIQUID CRYSTALS*. ISSN 1542-1406, 2018, vol. 660, no. 1, pp. 10-16., Registrované v: WOS
2. [1.1] LIU, Yun - LI, Xiaochuan - MIN, Kyeong Su - SON, Young-A. Emission behavior of naphthalimide-coumarin cassette. In *MOLECULAR CRYSTALS AND LIQUID CRYSTALS*. ISSN 1542-1406, 2018, vol. 662, no. 1, pp. 139-146., Registrované v: WOS
3. [1.1] SANATI, Soheila - REZVANI, Zolfaghar. Co-intercalation of Acid Red-27/sodium dodecyl sulfate in a Ce-containing Ni-Al-layered double hydroxide matrix and characterization of its luminescent properties. In *JOURNAL OF MOLECULAR LIQUIDS*. ISSN 0167-7322, 2018, vol. 249, no., pp. 318-325., Registrované v: WOS
4. [1.1] SOHMYA, Minoru - NAKAMURA, Takanori - SUGAHARA, Yoshiyuki - OGAWA, Makoto. Distribution Control-Oriented Intercalation of a Cationic Metal Complex into Layered Silicates Modified with Organosulfonic-Acid Moieties. In *LANGMUIR*. ISSN 0743-7463, 2018, vol. 34, no. 16, pp. 4762-4773., Registrované v: WOS
5. [1.1] TSUKAMOTO, Takamasa - SHIMADA, Tetsuya - TAKAGI, Shinsuke. Artificial Photosynthesis Model: Photochemical Reaction System with Efficient Light-Harvesting Function on Inorganic Nanosheets. In *ACS OMEGA*. ISSN 2470-1343, 2018, vol. 3, no. 12, pp. 18563-18571., Registrované v: WOS

ADCA17 BENCO, Ľubomír - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol - JÁNÉ, Eduard - VELIČ, Dušan. Europium-doped LaSi₃N₅ ternary nitride: synthesis, spectroscopy, computed electronic structure and band gaps. In *Journal of the American Ceramic Society*, 2011, vol. 94, no. 12, p. 4345-4351. (2010: 2.169 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0002-7820.

Citácie:

1. [1.1] PRIYANGA, G. Sudha - THOMAS, Tiju. Direct band gap narrowing and light-harvesting-potential in orthorhombic In-doped-AlFeO₃ perovskite: A first principles study. In *JOURNAL OF ALLOYS AND COMPOUNDS*. ISSN 0925-8388, 2018, vol. 750, no., pp. 312-319., Registrované v: WOS

ADCA18 BENEDEK, R. - THACKERAY, M. M. - LOW, J. - BUČKO, Tomáš. Simulation of aqueous dissolution of lithium manganate spinel from first principles. In *Journal of Physical Chemistry C*, 2012, vol. 116, no. 6, p. 4050-4059. (2011: 4.805 - IF, 2.320 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 1932-7447.

Citácie:

1. [1.1] KLYUKIN, Konstantin - ROSSO, Kevin M. - ALEXANDROV, Vitaly. Iron Dissolution from Goethite (alpha-FeOOH) Surfaces in Water by Ab Initio Enhanced Free-Energy Simulations. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 28, pp. 16086-16091., Registrované v: WOS
2. [1.1] KWON, Yonguk - LEE, Yongho - KIM, Sang-Ok - KIM, Hyung-Seok - KIM, Ki Jae - BYUN, Dongjin - CHOI, Wonchang. Conducting Polymer Coating on a High-Voltage Cathode Based on Soft Chemistry Approach toward Improving Battery Performance. In *ACS APPLIED MATERIALS & INTERFACES*. ISSN 1944-8244, 2018, vol. 10, no. 35, pp. 29457-29466., Registrované v: WOS
3. [1.1] NOMURA, Fumihito - LIU, Yubin - TANABE, Toyokazu - GUNJI, Takao - TSUDA, Takashi - UGAWA, Shinsaku - LEE, Hojin - OHSAKA, Takeo - MATSUMOTO, Futoshi. Elucidation of key factors of water-resistance of Li-rich solid-solution layered oxide cathode materials applicable to a water-based cathode preparation process for Li-ion battery. In *ELECTROCHIMICA ACTA*. ISSN 0013-4686, 2018, vol. 283, no., pp. 478-487., Registrované v: WOS
4. [1.1] SHEN, Zhizhang - KERISIT, Sebastien N. - STACK, Andrew G. - ROSSO, Kevin M. Free-Energy Landscape of the Dissolution of Gibbsite at High pH. In *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*. ISSN 1948-7185, 2018, vol. 9, no. 7, pp. 1809-1814., Registrované v: WOS
5. [1.1] ULLAH, Arslan - MAJID, Abdul - RANI, Naema. A review on first principles based studies for improvement of cathode material of lithium ion batteries. In *JOURNAL OF ENERGY CHEMISTRY*. ISSN 2095-4956, 2018, vol. 27, no. 1, pp. 219-237., Registrované v: WOS
6. [1.1] YU, Xiankai - CHEN, Xiao - BUCHHOLZ, D. Bruce - LI, Qianqian - WU, Jinsong - FENTER, Paul A. - BEDZYK, Michael J. - DRAVID, Vinayak P. - BARNETT, Scott A. Pulsed Laser Deposition and Characterization of Heteroepitaxial LiMn₂O₄/La_{0.5}Sr_{0.5}CoO₃ Bilayer Thin Films as Model Lithium Ion Battery Cathodes. In *ACS APPLIED NANO MATERIALS*. ISSN 2574-0970, 2018, vol. 1, no. 2, pp. 642-653., Registrované v: WOS

7. [1.1] ZHAN, Chun - WU, Tianpin - LU, Jun - AMINE, Khalil. Dissolution, migration, and deposition of transition metal ions in Li-ion batteries exemplified by Mn-based cathodes a critical review. In *ENERGY & ENVIRONMENTAL SCIENCE*. ISSN 1754-5692, 2018, vol. 11, no. 2, pp. 243-257., Registrované v: WOS

8. [1.1] ZHENG, Xueying - LIU, Weijie - QU, Qunting - SHI, Qiang - ZHENG, Honghe - HUANG, Yunhui. Effectively stabilizing 5 V spinel LiNi_{0.5}Mn_{1.5}O₄ cathode in organic electrolyte by polyvinylidene fluoride coating. In *APPLIED SURFACE SCIENCE*. ISSN 0169-4332, 2018, vol. 455, no., pp. 349-356., Registrované v: WOS

ADCA19 BENEDICT, Hans - SHENDEROVICH, Ilja G. - MALKINA, Oľga - MALKIN, Vladimír - DENISOV, Gleb S. - GOLUBEV, Nikolai S. - LIMBACH, Hans-Heinrich. Nuclear scalar spin-spin couplings and geometries of hydrogen bonds. In *Journal of the American Chemical Society*, 2000, vol. 122, no. 9, p. 1979-1988. ISSN 0002-7863.

Citácie:

1. [1.1] LAKSHMIPRIYA, A. - CHAUDHARY, Madhusudan - MOGURAMPELLE, Santosh - KLEIN, Michael L. - SURYAPRAKASH, N. Intramolecular Hydrogen Bonding Appetency for Conformational Penchants in Oxalohydrazide Fluoro Derivatives: NMR, MD, QTAIM, and NCI Studies. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 10, pp. 2703-2713., Registrované v: WOS

ADCA20 BERNARDO, E. - FIOCCO, L. - PRNOVÁ, Anna - KLEMENT, Róbert - GALUSEK, Dušan. Gehlenite: Eu³⁺ phosphors from a silicone resin and nano-sized fillers. In *Optical Materials*, 2014, vol. 36, no. 7, p. 1243-1249. (2013: 2.075 - IF, 0.766 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 0925-3467.

Citácie:

1. [1.1] FU, Shengyang - LIU, Wei - LIU, Shiwei - ZHAO, Shichang - ZHU, Yufang. 3D printed porous beta-Ca₂SiO₄ scaffolds derived from preceramic resin and their physicochemical and biological properties. In *SCIENCE AND TECHNOLOGY OF ADVANCED MATERIALS*. ISSN 1468-6996, 2018, vol. 19, no. 1, pp. 495-506., Registrované v: WOS

2. [1.1] PAN, Xiaolin - ZHANG, Di - WU, Yan - YU, Haiyan. Synthesis and characterization of calcium aluminate compounds from gehlenite by high-temperature solid-state reaction. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 12, pp. 13544-13550., Registrované v: WOS

3. [1.1] SHIH, Shao-Ju - CHOU, Yu-Jen - HADUSH, Abadi - LIN, Shih-Heng - HSIAO, Chih-Wei. Morphology Control of Eu-Doped Amorphous Gehlenite Phosphors Prepared by Spray Pyrolysis. In *JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY*. ISSN 1533-4880, 2018, vol. 18, no. 8, pp. 5849-5853., Registrované v: WOS

ADCA21 BISHOP, J.L. - MADEJOVÁ, Jana - KOMADEL, Peter - FRÖSCHL, H. The influence of structural Fe, Al and Mg on the infrared OH bands in spectra of dioctahedral smectites. In *Clay Minerals*, 2002, vol. 37, no. 4, p. 607-616. (2001: 0.610 - IF, karentované - CCC). (2002 - Current Contents). ISSN 0009-8558.

Citácie:

1. [1.1] ACKISS, S. - HORGAN, B. - SEELOS, F. - FARRAND, W. - WRAY, J. Mineralogic evidence for subglacial volcanism in the Sisyphi Montes region of Mars. In *ICARUS*. ISSN 0019-1035, 2018, vol. 311, no., pp. 357-370., Registrované v: WOS

2. [1.1] CHATTORAJ, Shovan L. - BANERJEE, Santanu - VAN DER MEER, Freek - RAY, P. K. Champati. Application of visible and infrared spectroscopy for the evaluation of evolved glauconite. In *INTERNATIONAL JOURNAL OF APPLIED EARTH OBSERVATION AND GEOINFORMATION*. ISSN 0303-2434, 2018, vol. 64, no., pp. 301-310., Registrované v: WOS

3. [1.1] HUANG, Liuqin - FENG, Can - JIANG, Hongchen - DONG, Hailiang - LIU, Zizhang - ZENG, Qiang - WANG, Xi - ZHANG, Li. Reduction of structural Fe(III) in nontronite by thermophilic microbial consortia enriched from hot springs in Tengchong, Yunnan Province, China. In *CHEMICAL GEOLOGY*. ISSN 0009-2541, 2018, vol. 479, no., pp. 47-57., Registrované v: WOS

4. [1.1] JIANG, Jun - CAO, Jinzhen - WANG, Wang - MEI, Changtong. Analysis on the Influence of Component Ratio on Properties of Silica/Montmorillonite Nanocomposites. In *MATERIALS*. ISSN 1996-1944, 2018, vol. 11, no. 11, pp., Registrované v: WOS

5. [1.1] PAN, Lu - EHLMANN, Bethany L. Aqueous Processes From Diverse Hydrous Minerals in the Vicinity of Amazonian-Aged Lyot Crater. In *JOURNAL OF GEOPHYSICAL RESEARCH-PLANETS*. ISSN 2169-9097, 2018, vol. 123, no. 7, pp. 1618-1648., Registrované v: WOS

6. [1.1] PELAYO, M. - MARCO, J. F. - FERNANDEZ, A. M. - VERGARA, L. - MELON, A. M. - PEREZ DEL VILLAR, L. Infrared and Mossbauer spectroscopy of Fe-rich smectites from Morron de Mateo bentonite deposit (Spain). In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 1, pp. 17-28., Registrované v: WOS

7. [1.1] SRIVASTAVA, Priyeshu - SIDDIAH, N. Siva - SANGODE, S. J. - MESHAM, D. C. Mineralogy and geochemistry of various colored bores from the Deccan volcanic province: Implications for paleoweathering and paleoenvironmental conditions. In *CATENA*. ISSN 0341-8162, 2018, vol. 167, no., pp. 44-59., Registrované v: WOS

8. [1.1] TSANTOS, C. - GIONIS, V. - CHRYSSIKOS, G. D. Smectite in bentonite: Near infrared systematics and estimation of layer charge. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 160, no., pp. 81-87., Registrované v: WOS

ADCA22 BLUGAN, Gurdial - MICHÁLKOVÁ, Monika - HNATKO, Miroslav - ŠAJGALÍK, Pavol - MINGHETTI, Tiziano - SCHELLE, Christian - GRAULE, Thomas - KUEBLER, Jakob. Processing and properties of alumina-carbon nano fibre ceramic composites using standard ceramic technology. In *Ceramics International*, 2011, vol. 37, no. 8, p. 3371-3379. (2010: 1.471 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] YU, Hui - HOU, Zhenhao - GUO, Xiaodong - CHEN, Yongjun - LI, Jianlin - LUO, Lijie - LI, Jianbao - YANG, Tao. Finite element analysis on flexural strength of Al₂O₃-ZrO₂ composite ceramics with different proportions. In *MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING*. ISSN 0921-5093, 2018, vol. 738, no., pp. 213-218., Registrované v: WOS

ADCA23 BOČA, Miroslav - JAMESON, Reginald F. - LINERT, Wolfgang. Fascinating variability in the

chemistry and properties of 2,6-bis-(benzimidazol-2-yl)-pyridine and 2,6-bis-(benzthiazol-2-yl)-pyridine and their complexes. In *Coordination Chemistry Reviews*, 2011, vol. 255, n. 1-2, p. 290-317. (2010: 10.018 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0010-8545.

Citácie:

1. [1.1] GUAN, David - THOMPSON, John R. - LEZNOFF, Daniel B. Emissive and birefringent Hg(CN)(2)-based coordination polymer materials with very distorted coordination geometries. In *CANADIAN JOURNAL OF CHEMISTRY*. ISSN 0008-4042, 2018, vol. 96, no. 2, pp. 226-234., Registrované v: WOS

2. [1.1] MAITY, Apurba - SIL, Amit - PATRA, Sanjib K. Ruthenium(II) Complexes of 4'-(Aryl)-2,2':6':2'-terpyridyl Ligands as Simple Catalysts for the Transfer Hydrogenation of Ketones. In *EUROPEAN JOURNAL OF INORGANIC CHEMISTRY*. ISSN 1434-1948, 2018, vol., no. 36, pp. 4063-4073., Registrované v: WOS

ADCA24 BOČA, Miroslav - BARAN, Peter - BOČA, Roman - KICKELBICK, Guido - RENZ, Franz - LINERT, Wolfgang. Imidazolidine ring-formation/cleavage due to intracomplex coordinative activation. In *Inorganic Chemistry Communications*, 1999, vol. 2, no. 5, p. 188-190.

Citácie:

1. [1.1] CHAHAL, Manoj - MANI, Kalaikodikumaran - LODHI, Chetan Singh - BUTCHER, Ray J. - RAJE, Sakthi - ANGAMUTHU, Raja. Metal Dependent Formation of Imidazolidine or Hemiaminal Ether Complexes from Multicomponent One-pot Reactions. In *CHEMISTRYSELECT*. ISSN 2365-6549, 2018, vol. 3, no. 34, pp. 9960-9964., Registrované v: WOS

ADCA25 BOČA, Miroslav - BARAN, Peter - BOČA, Roman - FUESS, H. - KICKELBICK, Guido - LINERT, Wolfgang - RENZ, Franz - SVOBODA, Ingrid. Selective imidazolidine ring-opening during complex formation of iron(III), copper(II), and zinc(II) with a multidentate ligand obtained from 2-pyridinecarboxaldehyde N-oxide and triethylenetetramine. In *Inorganic Chemistry*, 2000, vol. 39, no. 15, p. 3205-3212. ISSN 0020-1669.

Citácie:

1. [1.1] CHAHAL, Manoj - MANI, Kalaikodikumaran - LODHI, Chetan Singh - BUTCHER, Ray J. - RAJE, Sakthi - ANGAMUTHU, Raja. Metal Dependent Formation of Imidazolidine or Hemiaminal Ether Complexes from Multicomponent One-pot Reactions. In *CHEMISTRYSELECT*. ISSN 2365-6549, 2018, vol. 3, no. 34, pp. 9960-9964., Registrované v: WOS

2. [1.1] ZHAI, Feng - JORDAN, Richard F. Complexation of an indole-based alpha-aminoimine ligand to Pd(II). In *INORGANICA CHIMICA ACTA*. ISSN 0020-1693, 2018, vol. 482, no., pp. 491-496., Registrované v: WOS

ADCA26 BOČA, Miroslav - SVOBODA, Ingrid - RENZ, Franz - FUESS, H. Poly [methylammonium tris(μ₂-formato-K₂ O:O)cobalt(II)]. In *Acta Crystallographica Section C. Crystal Structure Communications*, 2004, vol. 60, p. M631-M633. (2004 - Current Contents). ISSN 0108-2701.

Citácie:

1. [1.1] MAZZUCA, Lidia - CANADILLAS-DELGADO, Laura - FABELLO, Oscar - ALBERTO RODRIGUEZ-VELAMAZAN, J. - LUZON, Javier - VALLCORBA, Oriol - SIMONET, Virginie - COLIN, Claire V. - RODRIGUEZ-CARVAJAL, Juan. Microscopic Insights on the Multiferroic Perovskite-Like [CH₃NH₃][Co(COOH)(3)] Compound. In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 2, pp. 388-399., Registrované v: WOS

ADCA27 BOČA, Miroslav - VALKO, M. - KICKELBICK, Guido - ĎURÍK, M. - LINERT, Wolfgang. CuII complexes with the new Schiff base ligands as a mono- and bis-condensation products of 2-pyridinecarboxaldehyde-N-oxide with diethylenetriamine. In *Inorganica Chimica Acta*, 2003, vol. 349, p. 111-122. ISSN 0020-1693.

Citácie:

1. [1.1] GURICOVA, Miroslava - PIZL, Martin - SMEKAL, Zdenek - NADHERNY, Ladislav - CEJKA, Jan - EIGNER, Vaclav - HOSKOVCOVA, Irena. Template synthesis and structure of Co(II), Ni(II), and Cu(II) complexes with pyridoxilydenetaurinate Schiff base ligand. In *INORGANICA CHIMICA ACTA*. ISSN 0020-1693, 2018, vol. 477, no., pp. 248-256., Registrované v: WOS

ADCA28 BOČA, Miroslav - BARBORÍK, Peter - MIČUŠÍK, Matej - OMASTOVÁ, Mária. X-ray photoelectron spectroscopy as detection tool for coordinated or uncoordinated fluorine atoms demonstrated on fluoride systems NaF, K₂TaF₇, K₃TaF₈, K₂ZrF₆, Na₇Zr₆F₃₁ and K₃ZrF₇. In *Solid State Sciences*, 2012, vol. 14, p. 828 - 832. (2011: 1.856 - IF, 0.800 - SJR, karentované - CCC). (2012 - Current Contents, WOS, SCOPUS). ISSN 1293-2558.

Citácie:

1. [1.1] NIE, K. - YANG, H.P. - GAO, Z. - WU, J.M. Fe-modified perovskite-type NaMgF₃ photocatalyst: Synthesis and photocatalytic properties. In *MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING*. ISSN 1369-8001, AUG 15 2018, vol. 83, p. 12-17., Registrované v: WOS

ADCA29 BOČA, Roman - BOČA, Miroslav - DLHÁŇ, L. - FALK, K. - FUESS, H. - HAASE, Wolfgang - JAROŠČIAK, R. - PAPÁNKOVÁ, B. - RENZ, Franz - VRBOVÁ, M. - WERNER, Rüdiger. Strong cooperativeness in the mononuclear iron(II) derivative exhibiting an abrupt spin transition above 400 K. In *Inorganic Chemistry*, 2001, vol. 40, no. 13, p. 3025-3033. ISSN 0020-1669.

Citácie:

1. [1.1] PAVLIK, Jan - LINARES, Jorge. Microscopic models of spin crossover. In *COMPTES RENDUS CHIMIE*. ISSN 1631-0748, 2018, vol. 21, no. 12, pp. 1170-1178., Registrované v: WOS

ADCA30 BOČA, Roman - BOČA, Miroslav - GEMBIČKÝ, Milan - JÄGER, Lothar - WAGNER, Christoph - FUESS, H. Versatile coordination mode of dicyanamide in nickel(II) complexes containing polyamines as blocking ligands. In *Polyhedron*, 2004, vol. 23, no. 15, p. 2337-2348. ISSN 0277-5387.

Citácie:

1. [1.1] PURKAYASTHA, Atanu - DEBNATH, Diptanu - MAJUMDER, Moumita - ORTEGA-CASTRO, Joaquin - KIRILLOV, Alexander M. - GANGULY, Rakesh - KLAKE, Julia - FRONTERA, Antonio - MISRA, Tarun Kumar. Nickel(II) based homo- vs

heterometallic 1D coordination polymers derived from a novel 6-aminouracil building block: Structures, topologies, non-covalent interactions, magnetism, and antibacterial activity. In INORGANICA CHIMICA ACTA. ISSN 0020-1693, 2018, vol. 482, no., pp. 384-394., Registrované v: WOS

- ADCA31 BOČA, Roman - RENZ, Franz - BOČA, Miroslav - FUESS, H. - HAASE, Wolfgang - KICKELBICK, Guido - LINERT, Wolfgang - VRBOVÁ-SCHIKORA, Martina. Tuning the spin crossover above room temperature: iron(II) complexes of substituted and deprotonated 2,6-bis(benzimidazol-2-yl)pyridine. In Inorganic Chemistry Communications, 2005, vol. 8, no. 2, p. 227-230.

Citácie:

1. [1.1] BARTUAL-MURGUI, Carlos - DIEGO, Rosa - VELA, Sergi - TEAT, Simon J. - ROUBEAU, Olivier - AROMI, Guillem. A Spin-Crossover Molecular Material Describing Four Distinct Thermal Pathways. In INORGANIC CHEMISTRY. ISSN 0020-1669, 2018, vol. 57, no. 17, pp. 11019-11026., Registrované v: WOS

- ADCA32 BODIŠOVÁ, Katarína - GALUSEK, Dušan - ŠVANČÁREK, Peter - POUCHLÝ, Václav - MACA, Karel. Grain growth suppression in alumina via doping and two-step sintering. In Ceramics International, 2015, vol. 41, no. 9, p. 11975-11983. (2014: 2.605 - IF, Q1 - JCR, 0.871 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] ARANTES, V. L. - NETO, A. L. P. - SILVEIRA, S. Two-Step Sintering of Alumina/Zirconia Functionally Graded Materials. In PRAKTISCHE METALLOGRAFIE-PRACTICAL METALLOGRAPHY. ISSN 0032-678X, 2018, vol. 55, no. 5, pp. 303-318., Registrované v: WOS

2. [1.1] OZTURK, Zeynep Taslicukur - KUSKONMAZ, Nilgun. The grain growth in alumina compacts sintered under high pressure. In INTERNATIONAL JOURNAL OF MATERIALS RESEARCH. ISSN 1862-5282, 2018, vol. 109, no. 12, pp. 1172-1175., Registrované v: WOS

3. [1.1] SEQUEIRA, S. I. H. - MONTEIRO, R. C. C. Sintering behaviour of a ZnO waste powder obtained as by-product from brass smelting. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 6, pp. 6250-6256., Registrované v: WOS

4. [1.1] YAN, Shiyu - YIN, Zengbin - YUAN, Juntang - XU, Weiwei - CHEN, Mingdan - YE, Jiadong. Microstructure and properties of submicron grained alumina ceramic tool material prepared by two-step microwave sintering. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 14, pp. 17479-17485., Registrované v: WOS

- ADCA33 BODIŠOVÁ, Katarína - KLEMENT, Róbert - GALUSEK, Dušan - POUCHLÝ, Václav - DRDLÍK, Daniel - MACA, Karel. Luminescent rare-earth-doped transparent alumina ceramics. In Journal of the European Ceramic Society, 2016, vol. 36, no. 12, p. 2975-2980. (2015: 2.933 - IF, Q1 - JCR, 1.150 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0955-2219.

Citácie:

1. [1.1] NAKAMURA, Takashi - OKAMURA, Shinya - NISHIDA, Hisataka - USAMI, Hirofumi - NAKANO, Yoshiro - WAKABAYASHI, Kazumichi - SEKINO, Tohru - YATANI, Hirofumi. Fluorescence of thulium-doped translucent zirconia. In DENTAL MATERIALS JOURNAL. ISSN 0287-4547, 2018, vol. 37, no. 6, pp. 1010-1016., Registrované v: WOS

2. [1.1] PENILLA, Elias H. - DEVIA-CRUZ, Luis F. - DUARTE, Matthew A. - HARDIN, Corey L. - KODERA, Yasuhiro - GARAY, Javier E. Gain in polycrystalline Nd-doped alumina: leveraging length scales to create a new class of high-energy, short pulse, tunable laser materials. In LIGHT-SCIENCE & APPLICATIONS. ISSN 2047-7538, 2018, vol. 7, no., pp., Registrované v: WOS

3. [1.1] YANG, Qinghua - JIANG, Benxue - CHEN, Shuilin - JIANG, Yiguang - ZHANG, Pande - WANG, Jun - XU, Shiqing - ZHANG, Long. Incorporation of Zn²⁺ ions into Al₂O₃:Er³⁺/Yb³⁺ transparent ceramics: An effective way to enhance upconversion and near infrared emission. In JOURNAL OF LUMINESCENCE. ISSN 0022-2313, 2018, vol. 199, no., pp. 45-52., Registrované v: WOS

- ADCA34 BODIŠOVÁ, Katarína - KAŠIAROVÁ, Monika - DOMANICKÁ, Magdaléna - HNATKO, Miroslav - LENČEŠ, Zoltán - VARCHULOVÁ NOVÁKOVÁ, Zuzana - VOJTAŠŠÁK, Ján - GROMOŠOVÁ, Silvia - ŠAJGALÍK, Pavol. Porous silicon nitride ceramics designed for bone substitute applications. In Ceramics International, 2013, vol. 39, p. 8355-8362. (2012: 1.789 - IF, 0.816 - SJR, karentované - CCC). (2013 - Current Contents, WOS, SCOPUS). ISSN 0272-8842.

Citácie:

1. [1.1] BOCK, Ryan M. - MARIN, Elia - RONDINELLA, Alfredo - BOSCHETTO, Francesco - ADACHI, Tetsuya - MCENTIRE, Bryan J. - BAL, B. Sonny - PEZZOTTI, Giuseppe. Development of a Si₃Al₂O₅N₂ glaze for improved osteoconductivity of implantable medical devices. In JOURNAL OF BIOMEDICAL MATERIALS RESEARCH PART B-APPLIED BIOMATERIALS. ISSN 1552-4973, 2018, vol. 106, no. 3, pp. 1084-1096., Registrované v: WOS

2. [1.1] HU, Shujuan - LI, Ang - FENG, Bo - TANG, Xiaoxia - ZHANG, Yue. A non-sintering fabrication method for porous Si₃N₄ ceramics via sol hydrothermal process. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 16, pp. 19699-19705., Registrované v: WOS

3. [1.1] LAL, Saurabh - CASELEY, Emily A. - HALL, Richard M. - TIPPER, Joanne L. Biological Impact of Silicon Nitride for Orthopaedic Applications: Role of Particle Size, Surface Composition and Donor Variation. In SCIENTIFIC REPORTS. ISSN 2045-2322, 2018, vol. 8, no., pp., Registrované v: WOS

4. [1.1] MA, Lijie - SONG, Yuehai - LI, Xiangming - LI, Rui - SHANG, Zhichao - WANG, Yixuan. Fabrication and properties of Si₃N₄ bioscaffolds with orderly-interconnected big pore channels and well-distributed small pores. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 10, pp. 11730-11736., Registrované v: WOS

5. [1.1] MOBBS, Ralph J. - RAO, Prashanth J. - PHAN, Kevin - HARDCASTLE, Philip - CHOY, Wen Jie - MCCARTNEY, Eric R. - DRUITT, Ross K. - MOUATT, Christopher A. L. - SORRELL, Charles C. Anterior Lumbar Interbody Fusion Using Reaction Bonded Silicon Nitride Implants: Long-Term Case Series of the First Synthetic Anterior Lumbar Interbody Fusion Spacer Implanted in Humans. In WORLD NEUROSURGERY. ISSN 1878-8750, 2018, vol. 120, no., pp. 256-264., Registrované v: WOS

- ADCA35 BODIŠOVÁ, Katarína - ŠAJGALÍK, Pavol - GALUSEK, Dušan - ŠVANČÁREK, Peter. Two-stage sintering of alumina with submicrometer grain size. In Journal of the American Ceramic Society, 2007,

vol. 90, no. 1, p. 330-332. (2006: 1.396 - IF, karentované - CCC). (2007 - Current Contents). ISSN 0002-7820.

Citácie:

1. [1.1] CHEN, Feng - YAN, Zhiqiao. Preparation of 3Y-TZP Nanoceramics by a Modified Two-Step Sintering with Ultrahigh Heating and Cooling Rates. In *ADVANCED FUNCTIONAL MATERIALS (CMC 2017)*, 2018, vol., no., pp. 651-659., Registrované v: WOS
 2. [1.1] CHEN, Ruoyuan - ZHOU, Jijun - ZHENG, Liang - ZHENG, Hui - ZHENG, Peng - YING, Zhihua - DENG, Jiangxia. Two-Step Sintering Behavior of Sol-Gel Derived Dense and Submicron-Grained YIG Ceramics. In *JOURNAL OF ELECTRONIC MATERIALS*. ISSN 0361-5235, 2018, vol. 47, no. 4, pp. 2411-2416., Registrované v: WOS
 3. [1.1] FARAG, S. - KONYASHIN, I. - RIES, B. The influence of grain growth inhibitors on the microstructure and properties of submicron, ultrafine and nano-structured hardmetals A review. In *INTERNATIONAL JOURNAL OF REFRACTORY METALS & HARD MATERIALS*. ISSN 0263-4368, 2018, vol. 77, no., pp. 12-30., Registrované v: WOS
 4. [1.1] GOLOVIN, Yu. I. - KORENKOV, V. V. - RAZLIVALOVA, S. S. - RODAEV, V. V. Physicomechanical Properties of Porous Zirconia Ceramics. In *RUSSIAN METALLURGY*. ISSN 0036-0295, 2018, vol., no. 10, pp. 961-967., Registrované v: WOS
 5. [1.1] LI, Lu - PU, Sanxu - LIU, Yuhang - ZHAO, Libin - MA, Ji - LI, Jiangong. High-purity disperse alpha-Al₂O₃ nanoparticles synthesized by high-energy ball milling. In *ADVANCED POWDER TECHNOLOGY*. ISSN 0921-8831, 2018, vol. 29, no. 9, pp. 2194-2203., Registrované v: WOS
 6. [1.1] OJAIMI, Christiane Lago - FERREIRA, Julieta Adriana - DOS SANTOS, Fabio Andre - CHINELATTO, Adilson Luiz - DE JESUS AGNOLON PALLONE, Eliria Maria - ANTONIO CHINELATTO, Adriana Scoton. Mechanical characterisation and hydrothermal degradation of Al₂O₃-15 % vol ZrO₂ nanocomposites consolidated by two-step sintering. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 14, pp. 16128-16136., Registrované v: WOS
 7. [1.1] PRAJZLER, Vladimir - SALAMON, David - MACA, Karel. Pressure-less rapid rate sintering of pre-sintered alumina and zirconia ceramics. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 9, pp. 10840-10846., Registrované v: WOS
 8. [1.1] SUN, Jialin - ZHAO, Jun - GONG, Feng - LI, Zuoli - NI, Xiuying. Design, fabrication and characterization of multi-layer graphene reinforced nanostructured functionally graded cemented carbides. In *JOURNAL OF ALLOYS AND COMPOUNDS*. ISSN 0925-8388, 2018, vol. 750, no., pp. 972-979., Registrované v: WOS
 9. [1.1] SUN, Jialin - ZHAO, Jun - NI, Xiuying - GONG, Feng - LI, Zuoli. Fabrication of dense nano-laminated tungsten carbide materials doped with Cr₃C₂/VC through two-step sintering. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 9, pp. 3096-3103., Registrované v: WOS
 10. [1.1] SUN, Jialin - ZHAO, Jun. Multi-layer graphene reinforced nano-laminated WC-Co composites. In *MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING*. ISSN 0921-5093, 2018, vol. 723, no., pp. 1-7., Registrované v: WOS
 11. [1.1] VARGAS-MARTINEZ, Nadia - DE JESUS RUIZ-BALTAZAR, Alvaro - MEDELLIN-CASTILLO, Nahum A. - YOBANNY REYES-LOPEZ, Simon. Synthesis of alpha-Alumina Nano-Onions by Thermal Decomposition of Aluminum Formate. In *JOURNAL OF NANOMATERIALS*. ISSN 1687-4110, 2018, vol., no., pp., Registrované v: WOS
 12. [1.1] ZHANG, Jiajie - ZHENG, Yong - CHEN, Jixin - ZHOU, Wei - ZHAO, Yijie - FENG, Ping. Microstructures and mechanical properties of Mo₂FeB₂-based cermets prepared by two-step sintering technique. In *INTERNATIONAL JOURNAL OF REFRACTORY METALS & HARD MATERIALS*. ISSN 0263-4368, 2018, vol. 72, no., pp. 56-62., Registrované v: WOS
 13. [1.1] ZHANG, Peng - WEI, Meng - WU, Kaituo - CHEN, Hongwei - ZHANG, Jihua. Two-step sintering for improving the energy storage properties of 0.8BaTiO₃-0.2BiYO₃ ceramics. In *JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS*. ISSN 0957-4522, 2018, vol. 29, no. 3, pp. 2471-2476., Registrované v: WOS
- ADCA36 BOKHAN, Denis - TEN-NO, Seichiro - NOGA, Jozef. Implementation of the CCSD(T)-F12 method using cusp conditions. In *Physical Chemistry Chemical Physics*, 2008, vol. 10, no. 23, p. 3320-3326. (2007: 3.343 - IF). ISSN 1463-9076.

Citácie:

1. [1.1] GYORFFY, Werner - WERNER, Hans-Joachim. Analytical energy gradients for explicitly correlated wave functions. II. Explicitly correlated coupled cluster singles and doubles with perturbative triples corrections: CCSD(T)-F12. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 11, pp., Registrované v: WOS
 2. [1.1] MA, Qianli - WERNER, Hans-Joachim. Explicitly correlated local coupled-cluster methods using pair natural orbitals. In *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*. ISSN 1759-0876, 2018, vol. 8, no. 6, pp., Registrované v: WOS
 3. [1.1] MA, Qianli - WERNER, Hans-Joachim. Scalable Electron Correlation Methods. 5. Parallel Perturbative Triples Correction for Explicitly Correlated Local Coupled Cluster with Pair Natural Orbitals. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 1, pp. 198-215., Registrované v: WOS
 4. [1.1] TEW, David P. - KATS, Daniel. Relaxing Constrained Amplitudes: Improved F12 Treatments of Orbital Optimization and Core-Valence Correlation Energies. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 11, pp. 5435-5440., Registrované v: WOS
- ADCA37 BREEN, Christopher - MADEJOVÁ, Jana - KOMADEL, Peter. Characterization of moderately acid-treated, size-fractionated montmorillonites using IR and MAS NMR-spectroscopy and thermal analysis. In *Journal of Materials Chemistry*, 1995, vol. 5, no. 3, p. 469-474. (1994: 1.520 - IF, karentované - CCC). (1995 - Current Contents). ISSN 0959-9428.

Citácie:

1. [1.1] ANTONIO CECILIA, Juan - PARDO, Laura - POZO, Manuel - BELLIDO, Eva - FRANCO, Francisco. Microwave-Assisted Acid Activation of Clays Composed of 2:1 Clay Minerals: A Comparative Study. In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 9, pp., Registrované v: WOS
2. [1.1] AYAT, Moulkheir - BELBACHIR, Mohammed - RAHMOUNI, Abdelkader. Cationic polymerization of poly(alpha-methylstyrene-block-isobutyl vinyl ether) using Maghnite-H⁺ clay (Algerian MMT) as catalyst. In *POLYMER BULLETIN*. ISSN

0170-0839, 2018, vol. 75, no. 12, pp. 5355-5371., Registrované v: WOS

3. [1.1] DUTTA, Dipak Kumar. Clay mineral catalysts. In SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 289-329., Registrované v: WOS

4. [1.1] MAHI, Ahmed - BELBACHIR, M. - AMMARI, Abdelkader - MEGHABER, R. - FERRAHI, M. I. Synthesis and characterization of poly(N-phenyl succinimide-thiophene) conducting polymer catalyzed by Maghnite-H+. In JOURNAL OF ELECTROANALYTICAL CHEMISTRY. ISSN 1572-6657, 2018, vol. 823, no., pp. 92-97., Registrované v: WOS

ADCA38 BREEN, Christopher - MADEJOVÁ, Jana - KOMADEL, Peter. Correlation of catalytic activity with infra-red, ²⁹Si MAS NMR and acidity data for HCl-treated fine fractions of montmorillonites. In Applied Clay Science, 1995, vol. 10, no. 3, p. 219-230. ISSN 0169-1317.

Citácie:

1. [1.1] ALASTAIR, Marsh - ANDREW, Heath - PASCALINE, Patureau - MARK, Evernden - PETE, Walker. Alkali activation behaviour of un-calcined montmorillonite and illite clay minerals. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 166, no., pp. 250-261., Registrované v: WOS

2. [1.1] FONSECA, Carla G. - VAISS, Viviane S. - WYPYCH, Fernando - DINIZ, Renata - LEITAO, Alexandre A. Investigation of the initial stages of the montmorillonite acid-activation process using DFT calculations. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 165, no., pp. 170-178., Registrované v: WOS

3. [1.1] JI, Shichao - ZHU, Jianxi - HE, Hongping - TAO, Qi - ZHU, Runliang - MA, Lingya - CHEN, Meng - LI, Shangying - ZHOU, Junming. Conversion of serpentine to smectite under hydrothermal condition: Implication for solid-state transformation. In AMERICAN MINERALOGIST. ISSN 0003-004X, 2018, vol. 103, no. 2, pp. 241-251., Registrované v: WOS

4. [1.1] LU, Yushen - DONG, Wenkai - WANG, Wenbo - DING, Junjie - WANG, Qin - HUI, Aiping - WANG, Aiqin. Optimal Synthesis of Environment-Friendly Iron Red Pigment from Natural Nanostructured Clay Minerals. In NANOMATERIALS. ISSN 2079-4991, 2018, vol. 8, no. 11, pp., Registrované v: WOS

5. [1.1] SIDORENKO, A. Yu. - KRAVTSOVA, A. V. - AHO, A. - HEINMAA, I. - KUZNETSOVA, T. F. - MURZIN, D. Yu. - AGABEKOV, V. E. Catalytic isomerization of alpha-pinene oxide in the presence of acid-modified clays. In MOLECULAR CATALYSIS. ISSN 2468-8231, 2018, vol. 448, no., pp. 18-29., Registrované v: WOS

ADCA39 BREEN, Christopher - WATSON, R. - MADEJOVÁ, Jana - KOMADEL, Peter - KLAPYTA, Z. Acid-activated organoclays: Preparation, characterization and catalytic activity of acid-treated tetraalkylammonium-exchanged smectites. In Langmuir, 1997, vol. 13, no. 24, p. 6473-6479. (1997 - Current Contents). ISSN 0743-7463.

Citácie:

1. [1.1] DI CREDICO, Barbara - COBANI, Elkid - CALLONE, Emanuela - CONZATTI, Lucia - CRISTOFORI, Davide - D'ARIENZO, Massimiliano - DIRE, Sandra - GIANNINI, Luca - HANEL, Thomas - SCOTTI, Roberto - STAGNARO, Paola - TADIELLO, Luciano - MORAZZONI, Franca. Size-controlled self-assembly of anisotropic sepiolite fibers in rubber nanocomposites. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 152, no., pp. 51-64., Registrované v: WOS

2. [1.1] DUTTA, Dipak Kumar. Clay mineral catalysts. In SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 289-329., Registrované v: WOS

3. [1.1] TLEUOV, A. S. - ARYSTANOVA, S. D. - LAVROV, B. A. - SHAPALOV, Sh K. - BAIYSBAY, O. P. - DOSBAYEVA, A. M. - MADYAROVA, Zh Zh. THE PHYSICO-CHEMICAL COMPOSITION OF THE NATURAL ALUMINOSILICATE SORBENTS USED FOR THE PHOSPHORUS EXTRACTION FROM PHOSPHORIC SLIME. In NEWS OF THE NATIONAL ACADEMY OF SCIENCES OF THE REPUBLIC OF KAZAKHSTAN-SERIES CHEMISTRY AND TECHNOLOGY. ISSN 2224-5286, 2018, vol., no. 2, pp. 44-51., Registrované v: WOS

ADCA40 BROSKA, Igor - RAVNA, Erling J. Krogh - VOJTKO, Peter - JANÁK, Marian - KONEČNÝ, Patrik - PENTRÁK, Martin - BAČÍK, Peter - LUPTÁKOVÁ, Jarmila - KULLERUD, K. Oriented inclusions in apatite in a post-UHP fluid-mediated regime (Tromsø Nappe, Norway). In European Journal of Mineralogy, 2014, vol. 26, p. 623-634. (2013: 1.506 - IF, 0.936 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 0935-1221.

Citácie:

1. [1.1] DONG, Jie - WEI, Chun-Jing - CLARKE, Geoffrey L. - ZHANG, Jian-Xin. Metamorphic Evolution During Deep Subduction and Exhumation of Continental Crust: Insights from Felsic Granulites in South Altyn Tagh, West China. In JOURNAL OF PETROLOGY. ISSN 0022-3530, 2018, vol. 59, no. 10, pp. 1965-1990., Registrované v: WOS

2. [1.1] JANOTS, Emilie - AUSTRHEIM, Hakon - SPANDLER, Carl - HAMMERLI, Johannes - TREPMANN, Claudia A. - BERNDT, Jasper - MAGNIN, Valerie - KEMP, Anthony I. S. Rare earth elements and Sm-Nd isotope redistribution in apatite and accessory minerals in retrogressed lower crust material (Bergen Arcs, Norway). In CHEMICAL GEOLOGY. ISSN 0009-2541, 2018, vol. 484, no., pp. 120-135., Registrované v: WOS

ADCA41 BRTÁŇOVÁ, Anna - MADEJOVÁ, Jana - BIZOVSKÁ, Valéria - KOMADEL, Peter. Utilization of near infrared spectroscopy for studying solvation properties of Cu-montmorillonites. In Spectrochimica Acta Part A - Molecular and Biomolecular Spectroscopy, 2014, vol. 123, p. 385-391. (2013: 2.129 - IF, 0.598 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 1386-1425.

Citácie:

1. [1.1] AFARANI, Zahra Ramazani - SARVI, Mehdi Nasiri - ALAVIJEH, Mozghan Akbari. Modification of montmorillonite nanolayers as a pH-responsive carrier of biomolecules: Delivery of vitamin B12. In JOURNAL OF THE TAIWAN INSTITUTE OF CHEMICAL ENGINEERS. ISSN 1876-1070, 2018, vol. 84, no., pp. 19-27., Registrované v: WOS

ADCA42 BUČKO, Tomáš - BENCO, Ľubomír - HAFNER, Jürgen - ÁNGYÁN, János G. Monomolecular cracking of propane over acidic chabazite: An ab initio molecular dynamics and transition path sampling study. In Journal of Catalysis, 2011, vol. 279, no. 1, p. 220-228. (2010: 5.415 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0021-9517.

Citácie:

1. [1.1] CHEN, Lin - FALSIG, Hanne - JANSSENS, Ton V. W. - GRONBECK, Henrik. Activation of oxygen on (NH₃-Cu-NH₃)(+) in NH₃-SCR over Cu-CHA. In *JOURNAL OF CATALYSIS*. ISSN 0021-9517, 2018, vol. 358, no., pp. 179-186., Registrované v: WOS
 2. [1.1] CNUUDE, Pieter - DE WISPELAERE, Kristof - VANDUYFHUYS, Louis - DEMUYNCK, Ruben - VAN DER MYNSBRUGGE, Jeroen - WAROQUIER, Michel - VAN SPEYBROECK, Veronique. How Chain Length and Branching Influence the Alkene Cracking Reactivity on H-ZSM-5. In *ACS CATALYSIS*. ISSN 2155-5435, 2018, vol. 8, no. 10, pp. 9579-9595., Registrované v: WOS
 3. [1.1] DE WISPELAERE, Kristof - VANDUYFHUYS, Louis - VAN SPEYBROECK, Veronique. Entropy Contributions to Transition State Modeling. In *MODELLING AND SIMULATION IN THE SCIENCE OF MICRO- AND MESO-POROUS MATERIALS*, 2018, vol., pp. 189-228., Registrované v: WOS
 4. [1.1] FANG, Hanjun - AWATI, Rohan - BOULFELFEL, Salah E. - RAVIKOVITCH, Peter I. - SHOLL, David S. First-Principles-Derived Force Fields for CH₄ Adsorption and Diffusion in Siliceous Zeolites. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 24, pp. 12880-12891., Registrované v: WOS
 5. [1.1] GRAJCIAR, Lukas - HEARD, Christopher J. - BONDARENKO, Anton A. - POLYNSKI, Mikhail V. - MEEPRASERT, Jittima - PIDKO, Evgeny A. - NACHTIGALL, Petr. Towards operando computational modeling in heterogeneous catalysis. In *CHEMICAL SOCIETY REVIEWS*. ISSN 0306-0012, 2018, vol. 47, no. 22, pp. 8307-8348., Registrované v: WOS
 6. [1.1] HAJEK, Julianna - CARATELLI, Chiara - DEMUYNCK, Ruben - DE WISPELAERE, Kristof - VANDUYFHUYS, Louis - WAROQUIER, Michel - VAN SPEYBROECK, Veronique. On the intrinsic dynamic nature of the rigid UiO-66 metal-organic framework. In *CHEMICAL SCIENCE*. ISSN 2041-6520, 2018, vol. 9, no. 10, pp. 2723-2732., Registrované v: WOS
 7. [1.1] KADAM, Shashikant A. - LI, Haoguang - WORMSBECHER, Richard F. - TRAVERT, Arnaud. Impact of Zeolite Structure on Entropic-Enthalpic Contributions to Alkane Monomolecular Cracking: An IR Operando Study. In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 21, pp. 5489-5492., Registrované v: WOS
 8. [1.1] RYBICKI, Marcin - SAUER, Joachim. Ab Initio Prediction of Proton Exchange Barriers for Alkanes at Bronsted Sites of Zeolite H-MFI. In *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*. ISSN 0002-7863, 2018, vol. 140, no. 51, pp. 18151-18161., Registrované v: WOS
 9. [1.1] VAN SANTEN, Rutger A. - LIU, Chong. Theory of Zeolite Catalysis: An Introductory Account. In *MODELLING AND SIMULATION IN THE SCIENCE OF MICRO- AND MESO-POROUS MATERIALS*, 2018, vol., no., pp. 151-188., Registrované v: WOS
 10. [1.1] VAN SANTEN, Rutger A. - SENGAR, Aditya - STEUR, Erik. The challenge of catalyst prediction. In *FARADAY DISCUSSIONS*. ISSN 1359-6640, 2018, vol. 208, no., pp. 35-52., Registrované v: WOS
- ADCA43 BUČKO, Tomáš - LEBÈGUE, Sébastien - ÁNGYÁN, János G. - HAFNER, Jürgen. Extending the applicability of the Tkatchenko-Scheffler dispersion correction via iterative Hirshfeld partitioning. In *Journal of Chemical Physics*, 2014, vol. 141, p. 034114-1-034114-17. (2013: 3.122 - IF, 1.532 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] BEDOYA-MARTINEZ, Natalia - GIUNCHI, Andrea - SALZILLO, Tommaso - VENUTI, Elisabetta - DELLA VALLE, Raffaele Guido - ZOJER, Egbert. Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 8, pp. 4380-4390., Registrované v: WOS
2. [1.1] BERAU, Tristan - DISTASIO, Robert A. - TKATCHENKO, Alexandre - VON LILIENFELD, O. Anatole. Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 24, pp., Registrované v: WOS
3. [1.1] FANG, Hanjun - AWATI, Rohan - BOULFELFEL, Salah E. - RAVIKOVITCH, Peter I. - SHOLL, David S. First-Principles-Derived Force Fields for CH₄ Adsorption and Diffusion in Siliceous Zeolites. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 24, pp. 12880-12891., Registrované v: WOS
4. [1.1] HESSELMANN, Andreas - MEITEI, Oinam Romesh. Intermolecular dispersion energies from coupled exact-exchange Kohn-Sham excitation energies and vectors. In *COMPUTATIONAL AND THEORETICAL CHEMISTRY*. ISSN 2210-271X, 2018, vol. 1129, no., pp. 57-69., Registrované v: WOS
5. [1.1] HIJAZI, Houssam - CANTREL, Laurent - PAUL, Jean-Francois. Reactivity of Silver Iodide (beta-AgI) Surfaces: A Density Functional Theory Study. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 46, pp. 26401-26408., Registrované v: WOS
6. [1.1] ISLAS-VARGAS, Claudia - GUEVARA-GARCIA, Alfredo - OLIVER-TOLENTINO, M. - RAMOS-SANCHEZ, G. - GONZALEZ, I. - GALVAN, Marcelo. Experimental and Theoretical Investigation on the Origin of the High Intercalation Voltage of K₂Zn₃[Fe(CN)₆](2) Cathode. In *JOURNAL OF THE ELECTROCHEMICAL SOCIETY*. ISSN 0013-4651, 2018, vol. 166, no. 3, pp. A5139-A5145., Registrované v: WOS
7. [1.1] LAO, Ka Un - HERBERT, John M. Atomic Orbital Implementation of Extended Symmetry-Adapted Perturbation Theory (XSAPT) and Benchmark Calculations for Large Supramolecular Complexes. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 6, pp. 2955-2978., Registrované v: WOS
8. [1.1] LIANG, Ting - CHEN, Wen-Qi - HU, Cui-E. - CHEN, Xiang-Rong - CHEN, Qi-Feng. Lattice dynamics and thermal conductivity of lithium fluoride via first-principles calculations. In *SOLID STATE COMMUNICATIONS*. ISSN 0038-1098, 2018, vol. 272, no., pp. 28-32., Registrované v: WOS
9. [1.1] LIU, Peng-Fei - BO, Tao - XU, Juping - YIN, Wen - ZHANG, Junrong - WANG, Fangwei - ERIKSSON, Olle - WANG, Bao-Tian. First-principles calculations of the ultralow thermal conductivity in two-dimensional group-IV selenides. In *PHYSICAL REVIEW B*. ISSN 2469-9950, 2018, vol. 98, no. 23, pp., Registrované v: WOS
10. [1.1] MOSYAGIN, Igor - GAMBINO, Davide - SANGIOVANNI, Davide G. - ABRIKOSOV, Igor A. - CAFFREY, Nuala M. Effect of dispersion corrections on ab initio predictions of graphite and diamond properties under pressure. In *PHYSICAL REVIEW B*. ISSN 2469-9950, 2018, vol. 98, no. 17, pp., Registrované v: WOS
11. [1.1] SROUR, Juliana - BADAWI, Michael - HASSAN, Fouad El Haj - POSTNIKOV, Andrei. Comparative study of structural and electronic properties of GaSe and InSe polytypes. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018,

vol. 149, no. 5, pp., Registrované v: WOS

12. [1.1] SUN, Minglei - CHOU, Jyh-Pin - SHI, Lihong - GAO, Junfeng - HU, Alice - TANG, Wencheng - ZHANG, Gang. Few-Layer PdSe₂ Sheets: Promising Thermoelectric Materials Driven by High Valley Convergence. In ACS OMEGA. ISSN 2470-1343, 2018, vol. 3, no. 6, pp. 5971-5979., Registrované v: WOS

13. [1.1] WANG, Da-Wei - WANG, Xiao-Hua - YANG, Ai-Jun - CHU, Ji-Feng - LV, Pin-Lei - LIU, Yang - RONG, Ming-Zhe. MoTe₂: A Promising Candidate for SF₆ Decomposition Gas Sensors With High Sensitivity and Selectivity. In IEEE ELECTRON DEVICE LETTERS. ISSN 0741-3106, 2018, vol. 39, no. 2, pp. 292-295., Registrované v: WOS

14. [1.1] WANG, Dawei - WANG, Xiaohua - YANG, Aijun - LV, Pinlei - CHU, Jifeng - LIU, Yang - RONG, Mingzhe - WANG, Chanqiong. A first principles theoretical study of the adsorption of SF₆ decomposition gases on a cassiterite (110) surface. In MATERIALS CHEMISTRY AND PHYSICS. ISSN 0254-0584, 2018, vol. 212, no., pp. 453-460., Registrované v: WOS

15. [1.1] WANG, Xiao Hua - WANG, Da Wei - YANG, Ai Jun - KORATKAR, Nikhil - CHU, Ji Feng - LV, Pin Lei - RONG, Ming Zhe. Effects of adatom and gas molecule adsorption on the physical properties of tellurene: a first principles investigation. In PHYSICAL CHEMISTRY CHEMICAL PHYSICS. ISSN 1463-9076, 2018, vol. 20, no. 6, pp. 4058-4066., Registrované v: WOS

16. [1.1] ZHANG, Yanhui - SANVITO, Stefano. First-principles investigation of the thermodynamic stability of MB₂ materials surfaces (M=Ti/Zr/Hf). In JOURNAL OF THE AMERICAN CERAMIC SOCIETY. ISSN 0002-7820, 2018, vol. 101, no. 9, pp. 4118-4127., Registrované v: WOS

17. [1.1] ZHAO, Qi-yi - GUO, Yaohui - ZHOU, Yixuan - YAO, Zehan - REN, Zhaoyu - BAI, Jintao - XU, Xinlong. Band alignments and heterostructures of monolayer transition metal trichalcogenides MX₃ (M = Zr, Hf; X = S, Se) and dichalcogenides MX₂ (M = Tc, Re; X = S, Se) for solar applications. In NANOSCALE. ISSN 2040-3364, 2018, vol. 10, no. 7, pp. 3547-3555., Registrované v: WOS

ADCA44 BUČKO, Tomáš - ŠIMKO, František. On the structure of crystalline and molten cryolite: Insights from the ab initio molecular dynamics in NpT ensemble. In Journal of Chemical Physics, 2016, vol. 144, no. 6, p. 064502-1-064502-10. (2015: 2.894 - IF, Q2 - JCR, 0.953 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] GHERIBI, Aimen E. - MACHADO, Kelly - ZANGHI, Didier - BESSADA, Catherine - SALANNE, Mathieu - CHARTRAND, Patrice. On the determination of ion transport numbers in molten salts using molecular dynamics. In ELECTROCHIMICA ACTA. ISSN 0013-4686, 2018, vol. 274, no., pp. 266-273., Registrované v: WOS

ADCA45 BUČKO, Tomáš - LEBÈGUE, Sébastien - GOULD, Tim - ÁNGYÁN, János G. Many-body dispersion corrections for periodic systems: an efficient reciprocal space implementation. In Journal of Physics: Condensed Matter, 2016, vol. 28, no. 4, p. 045201-1-045201-13. (2015: 2.209 - IF, Q2 - JCR, 0.824 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0953-8984.

Citácie:

1. [1.1] BEDOYA-MARTINEZ, Natalia - GIUNCHI, Andrea - SALZILLO, Tommaso - VENUTI, Elisabetta - DELLA VALLE, Raffaele Guido - ZOJER, Egbert. Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 8, pp. 4380-4390., Registrované v: WOS

2. [1.1] GRUBER, Thomas - GRUENEIS, Andreas. Ab initio calculations of carbon and boron nitride allotropes and their structural phase transitions using periodic coupled cluster theory. In PHYSICAL REVIEW B. ISSN 2469-9950, 2018, vol. 98, no. 13, pp., Registrované v: WOS

3. [1.1] HESSELMANN, Andreas. Geometry optimisations with a nonlocal density-functional theory method based on a double Hirshfeld partitioning. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 4, pp., Registrované v: WOS

4. [1.1] HOJA, Johannes - TKATCHENKO, Alexandre. First-principles stability ranking of molecular crystal polymorphs with the DFT plus MBD approach. In FARADAY DISCUSSIONS. ISSN 1359-6640, 2018, vol. 211, no., pp. 253-274., Registrované v: WOS

5. [1.1] KHALIL, Ibrahim - JABRAOUI, Hicham - MAURIN, Guillaume - LEBÈGUE, Sébastien - BADAWI, Michael - THOMAS, Karine - MAUGE, Françoise. Selective Capture of Phenol from Biofuel Using Protonated Faujasite Zeolites with Different Si/Al Ratios. In JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, 2018, vol. 122, no. 46, pp. 26419-26429., Registrované v: WOS

6. [1.1] LOBODA, Oleksandr A. - DOLGONOS, Goryoriy A. - BOESE, A. Daniel. Towards hybrid density functional calculations of molecular crystals via fragment-based methods. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 12, pp., Registrované v: WOS

7. [1.1] MOELLER, Andreas - KONZE, Philipp M. - DRONSKOWSKI, Richard. High-Pressure Behavior of Lead Cyanamide PbNCN. In ZEITSCHRIFT FÜR ANORGANISCHE UND ALLGEMEINE CHEMIE. ISSN 0044-2313, 2018, vol. 644, no. 24, pp. 1881-1885., Registrované v: WOS

8. [1.1] REIMERS, Jeffrey R. - TAWFIK, Sherif Abdulkader - FORD, Michael J. van der Waals forces control ferroelectric-antiferroelectric ordering in CuInP₂S₆ and CuBiP₂Se₆ laminar materials. In CHEMICAL SCIENCE. ISSN 2041-6520, 2018, vol. 9, no. 39, pp. 7620-7627., Registrované v: WOS

9. [1.1] SROUR, Juliana - BADAWI, Michael - HASSAN, Fouad El Haj - POSTNIKOV, Andrei. Comparative study of structural and electronic properties of GaSe and InSe polytypes. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 5, pp., Registrované v: WOS

10. [1.1] TAWFIK, Sherif Abdulkader - REIMERS, Jeffrey R. - STAMPFL, Catherine - FORD, Michael J. van der Waals Forces Control the Internal Chemical Structure of Monolayers within the Lamellar Materials CuInP₂S₆ and CuBiP₂Se₆. In JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, 2018, vol. 122, no. 39, pp. 22675-22687., Registrované v: WOS

11. [1.1] VARGA, Stefan. Communication: Renormalization method for infinite lattice sums revisited: Lattice sums with Bloch phase factors. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 5, pp., Registrované v: WOS

12. [1.1] WIEME, J. - LEJAEGHERE, K. - KRESSE, G. - VAN SPEYBROECK, V. Tuning the balance between dispersion and entropy to design temperature-responsive flexible metal-organic frameworks. In NATURE COMMUNICATIONS. ISSN 2041-1723, 2018, vol. 9, no., pp., Registrované v: WOS

- ADCA46 BUČKO, Tomáš - CHIBANI, Siwar - PAUL, Jean-François - CANTREL, Laurent - BADAWI, Michael. Dissociative iodomethane adsorption on Ag-MOR and the formation of AgI clusters: an ab initio molecular dynamics study. In *Physical Chemistry Chemical Physics*, 2017, vol. 19, no., p. 27530-27543. (2016: 4.123 - IF, Q1 - JCR, 1.685 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 1463-9076.

Citácie:

1. [1.1] GRAJCIAR, Lukas - HEARD, Christopher J. - BONDARENKO, Anton A. - POLYNSKI, Mikhail V. - MEEPRASERT, Jittima - PIDKO, Evgeny A. - NACHTIGALL, Petr. Towards operando computational modeling in heterogeneous catalysis. In *CHEMICAL SOCIETY REVIEWS*. ISSN 0306-0012, 2018, vol. 47, no. 22, pp. 8307-8348., Registrované v: WOS
2. [1.1] HUVE, Joffrey - RYZHIKOV, Andrey - NOUALI, Habiba - LALIA, Virginie - AUGÉ, Gregoire - DAOU, T. Jean. Porous sorbents for the capture of radioactive iodine compounds: a review. In *RSC ADVANCES*. ISSN 2046-2069, 2018, vol. 8, no. 51, pp. 29248-29273., Registrované v: WOS

- ADCA47 BUČKO, Tomáš - LEBÈGUE, Sébastien - HAFNER, Jürgen - ÁNGYÁN, János G. Improved density dependent correction for the description of London dispersion forces. In *Journal of Chemical Theory and Computation*, 2013, vol. 9, no. 10, p. 4293-4299. (2012: 5.389 - IF, 2.744 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 1549-9618.

Citácie:

1. [1.1] BEDOYA-MARTINEZ, Natalia - GIUNCHI, Andrea - SALZILLO, Tommaso - VENUTI, Elisabetta - DELLA VALLE, Raffaele Guido - ZOJER, Egbert. Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 8, pp. 4380-4390., Registrované v: WOS
2. [1.1] CHEN, Dachang - ZHANG, Xiaoxing - TANG, Ju - FANG, Jiani - LI, Yi - LIU, Huijun. Adsorption and dissociation mechanism of SO₂ and H₂S on Pt decorated graphene: a DFT-D3 study. In *APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING*. ISSN 0947-8396, 2018, vol. 124, no. 6, pp., Registrované v: WOS
3. [1.1] DOLGONOS, Grygoriy A. - LOBODA, Oleksandr A. - BOESE, A. Daniel. Development of Embedded and Performance of Density Functional Methods for Molecular Crystals. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 2, pp. 708-713., Registrované v: WOS
4. [1.1] HESSOU, Etienne - JABRAOUI, Hicham - CHEBBI, Mouheb - CHIBANI, Siwar - CANTREL, Laurent - BADAWI, Michael. Evaluation of the Inhibiting Effect of Organic Compounds on the Adsorption of Iodine Compounds in Cation-Exchanged Zeolites: A DFT Study. In *RECENT ADVANCES IN ENVIRONMENTAL SCIENCE FROM THE EURO-MEDITERRANEAN AND SURROUNDING REGIONS, VOLS I AND II*. ISSN 2522-8714, 2018, vol., no., pp. 107-109., Registrované v: WOS
5. [1.1] HIJAZI, Houssam - CANTREL, Laurent - PAUL, Jean-Francois. Reactivity of Silver Iodide (beta-AgI) Surfaces: A Density Functional Theory Study. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 46, pp. 26401-26408., Registrované v: WOS
6. [1.1] LI, Musen - REIMERS, Jeffrey R. - DOBSON, John F. - GOULD, Tim. Faraday cage screening reveals intrinsic aspects of the van der Waals attraction. In *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*. ISSN 0027-8424, 2018, vol. 115, no. 44, pp. E10295-E10302., Registrované v: WOS
7. [1.1] LIU, Peng-Fei - BO, Tao - XU, Juping - YIN, Wen - ZHANG, Junrong - WANG, Fangwei - ERIKSSON, Olle - WANG, Bao-Tian. First-principles calculations of the ultralow thermal conductivity in two-dimensional group-IV selenides. In *PHYSICAL REVIEW B*. ISSN 2469-9950, 2018, vol. 98, no. 23, pp., Registrované v: WOS
8. [1.1] MARCONDES, Michel L. - WENTZCOVITCH, Renata M. - ASSALI, Lucy V. C. Importance of van der Waals interaction on structural, vibrational, and thermodynamic properties of NaCl. In *SOLID STATE COMMUNICATIONS*. ISSN 0038-1098, 2018, vol. 273, no., pp. 11-16., Registrované v: WOS
9. [1.1] PIOTROWSKI, Mauricio J. - NAGURNIAK, Glaucio R. - DA SILVA, Eder H. - PARREIRA, Renato L. T. Bare versus protected tetrairidium clusters by density functional theory. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 46, pp. 29480-29492., Registrované v: WOS
10. [1.1] SROUR, Juliana - BADAWI, Michael - HASSAN, Fouad El Haj - POSTNIKOV, Andrei. Comparative study of structural and electronic properties of GaSe and InSe polytypes. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 5, pp., Registrované v: WOS
11. [1.1] SUN, Minglei - CHOU, Jyh-Pin - SHI, Lihong - GAO, Junfeng - HU, Alice - TANG, Wencheng - ZHANG, Gang. Few-Layer PdSe₂ Sheets: Promising Thermoelectric Materials Driven by High Valley Convergence. In *ACS OMEGA*. ISSN 2470-1343, 2018, vol. 3, no. 6, pp. 5971-5979., Registrované v: WOS
12. [1.1] WEN, Mingjian - CARR, Stephen - FANG, Shiang - KAXIRAS, Efthimios - TADMOR, Ellad B. Dihedral-angle-corrected registry-dependent interlayer potential for multilayer graphene structures. In *PHYSICAL REVIEW B*. ISSN 2469-9950, 2018, vol. 98, no. 23, pp., Registrované v: WOS
13. [1.1] ZHAO, Qi-yi - GUO, Yaohui - ZHOU, Yixuan - YAO, Zehan - REN, Zhaoyu - BAI, Jintao - XU, Xinlong. Band alignments and heterostructures of monolayer transition metal trichalcogenides MX₃ (M = Zr, Hf; X = S, Se) and dichalcogenides MX₂ (M = Tc, Re; X = S, Se) for solar applications. In *NANOSCALE*. ISSN 2040-3364, 2018, vol. 10, no. 7, pp. 3547-3555., Registrované v: WOS

- ADCA48 BUČKO, Tomáš - HAFNER, Jürgen - LEBÈGUE, Sébastien - ÁNGYÁN, János G. Spin crossover transition of Fe(phen)₂(NCS)₂: periodic dispersion-corrected density-functional study. In *Physical Chemistry Chemical Physics*, 2012, vol. 14, no. 16, p. 5389-5396. (2011: 3.573 - IF, 1.697 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 1463-9076.

Citácie:

1. [1.1] VELA, Sergi - PAULSEN, Hauke. Cooperativity in Spin Crossover Systems. An Atomistic Perspective on the Devil's Staircase. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 15, pp. 9478-9488., Registrované v: WOS
2. [1.1] WEN, Zhongqian - ZHOU, Liping - CHENG, Jue-Fei - LI, Shu-Jin - YOU, Wen-Long - WANG, Xuefeng. Spin crossover and high spin filtering behavior in Co-Pyridine and Co-Pyrimidine molecules. In *JOURNAL OF PHYSICS-CONDENSED*

MATTER. ISSN 0953-8984, 2018, vol. 30, no. 10, pp., Registrované v: WOS

3. [1.1] WOLNY, Juliusz A. - SCHUNEMANN, Volker - NEMETH, Zoltan - VANKO, Gyorgy. Spectroscopic techniques to characterize the spin state: Vibrational, optical, Mossbauer, NMR, and X-ray spectroscopy. In *COMPOTES RENDUS CHIMIE*. ISSN 1631-0748, 2018, vol. 21, no. 12, pp. 1152-1169., Registrované v: WOS

ADCA49 BUČKO, Tomáš - LEBÈGUE, Sébastien - HAFNER, Jürgen - ÁNGYÁN, János G. Tkatchenko-Scheffler van der Waals correction method with and without self-consistent screening applied to solids. In *Physical Review B*, 2013, vol. 87, no. 6, p. 064110-1-064110-15. (2012: 3.767 - IF, 3.159 - SJR, karentované - CCC). (2013 - Current Contents, WOS, SCOPUS). ISSN 1550-235X.

Citácie:

1. [1.1] BIJOY, T. K. - MURUGAN, P. - KUMAR, Vijay. Atomic structure and electronic properties of $A(2)B(2)XY$ ($A = \text{Si-Pb}$, $B = \text{Cl-I}$, and $XY = \text{PN}$ and SiS) inorganic double helices: first principles calculations. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 15, pp. 10060-10068., Registrované v: WOS

2. [1.1] CHA, Janghwan - SUNG, Dongchul - MIN, Kyung-Ah - HONG, Sukyun. Van der Waals Density Functional Theory Study of Molecular Adsorbates on MoX_2 ($X = \text{S, Se or Te}$). In *JOURNAL OF THE KOREAN PHYSICAL SOCIETY*. ISSN 0374-4884, 2018, vol. 73, no. 1, pp. 100-104., Registrované v: WOS

3. [1.1] CURUTCHET, Carles - CUPELLINI, Lorenzo - KONGSTED, Jacob - CORNI, Stefano - FREDIANI, Luca - STEINDAL, Arnfinn Hykkerud - GUIDO, Ciro A. - SCALMANI, Giovanni - MENNUCCI, Benedetta. Density-Dependent Formulation of Dispersion-Repulsion Interactions in Hybrid Multiscale Quantum/Molecular Mechanics (QM/MM) Models. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 3, pp. 1671-1681., Registrované v: WOS

4. [1.1] DE OLIVEIRA, J. B. - DE OLIVEIRA, I. S. S. - PADILHA, J. E. - MIWA, R. H. Tunable magnetism and spin-polarized electronic transport in graphene mediated by molecular functionalization of extended defects. In *PHYSICAL REVIEW B*. ISSN 2469-9950, 2018, vol. 97, no. 4, pp., Registrované v: WOS

5. [1.1] ELIAS, Badal H. - ILYAS, Bahaa M. - SAADI, Nawzat S. A first principle study of the perovskite lanthanum aluminate. In *MATERIALS RESEARCH EXPRESS*. ISSN 2053-1591, 2018, vol. 5, no. 8, pp., Registrované v: WOS

6. [1.1] FREIRE, Rafael L. H. - GUEDES-SOBRINHO, Diego - KIEJNA, Adam - DA SILVA, Juarez L. F. Comparison of the Performance of van der Waals Dispersion Functionals in the Description of Water and Ethanol on Transition Metal Surfaces. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 3, pp. 1577-1588., Registrované v: WOS

7. [1.1] HU, Chongze - NI, Peter - ZHAN, Li - ZHAO, Huijuan - HE, Jian - TRITT, Terry M. - HUANG, Jingsong - SUMPTER, Bobby G. Theoretical investigations of electrical transport properties in CoSb_3 skutterudites under hydrostatic loadings. In *RARE METALS*. ISSN 1001-0521, 2018, vol. 37, no. 4, pp. 316-325., Registrované v: WOS

8. [1.1] HUANG YAN - HU ZIYU - GONG XU - SHAO XIAOHONG. Structural, electronic and photocatalytic properties of atomic defective BiI_3 monolayers. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 691, no., pp. 341-346., Registrované v: WOS

9. [1.1] JAIMES, R. - CERVANTES-ALCALA, R. - GARCIA-GARCIA, W. - MIRANDA-HERNANDEZ, M. Ab initio computational modeling of the electrochemical reactivity of quinones on gold and glassy carbon electrodes. In *ELECTROCHIMICA ACTA*. ISSN 0013-4686, 2018, vol. 284, no., pp. 108-118., Registrované v: WOS

10. [1.1] KABAKOVA, Irina V. - AZURI, Ido - CHEN, Zhuoying - NAYAK, Pabitra K. - SNAITH, Henry J. - KRONIK, Leeor - PATERSON, Carl - BAKULIN, Artem A. - EGGER, David A. The effect of ionic composition on acoustic phonon speeds in hybrid perovskites from Brillouin spectroscopy and density functional theory. In *JOURNAL OF MATERIALS CHEMISTRY C*. ISSN 2050-7526, 2018, vol. 6, no. 15, pp. 3861-3868., Registrované v: WOS

11. [1.1] KHABIBULLIN, Artem R. - KAROLAK, Aleksandra - BUDZEVICH, Mikalai M. - MCLAUGHLIN, Mark L. - MORSE, David L. - WOODS, Lilia M. Structure and properties of DOTA-chelated radiopharmaceuticals within the Ac-225 decay pathway. In *MEDCHEMCOMM*. ISSN 2040-2503, 2018, vol. 9, no. 7, pp. 1155-1163., Registrované v: WOS

12. [1.1] KO, Hsin-Yu - DISTASIO, Robert A. - SANTRA, Biswajit - CAR, Roberto. Thermal expansion in dispersion-bound molecular crystals. In *PHYSICAL REVIEW MATERIALS*. ISSN 2475-9953, 2018, vol. 2, no. 5, pp., Registrované v: WOS

13. [1.1] LI, Jinyu - FLEURAT-LESSARD, Paul - ZAERA, Francisco - DELBECQ, Francoise. Switch in Relative Stability between cis and trans 2-Butene on $\text{Pt}(111)$ as a Function of Experimental Conditions: A Density Functional Theory Study. In *ACS CATALYSIS*. ISSN 2155-5435, 2018, vol. 8, no. 4, pp. 3067-+, Registrované v: WOS

14. [1.1] MARCONDES, Michel L. - WENTZCOVITCH, Renata M. - ASSALI, Lucy V. C. Importance of van der Waals interaction on structural, vibrational, and thermodynamic properties of NaCl . In *SOLID STATE COMMUNICATIONS*. ISSN 0038-1098, 2018, vol. 273, no., pp. 11-16., Registrované v: WOS

15. [1.1] MOSYAGIN, Igor - GAMBINO, Davide - SANGIOVANNI, Davide G. - ABRKOSOV, Igor A. - CAFFREY, Nuala M. Effect of dispersion corrections on ab initio predictions of graphite and diamond properties under pressure. In *PHYSICAL REVIEW B*. ISSN 2469-9950, 2018, vol. 98, no. 17, pp., Registrované v: WOS

16. [1.1] PIOTROWSKI, Mauricio J. - NAGURNIAK, Glaucio R. - DA SILVA, Eder H. - PARREIRA, Renato L. T. Bare versus protected tetrairidium clusters by density functional theory. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 46, pp. 29480-29492., Registrované v: WOS

17. [1.1] RERAT, Michel - PASCALE, Fabien - NOEL, Yves - CARBONNIERE, Philippe - DOVESI, Roberto. Scalars, vectors and tensors evolving from slabs to bulk. In *THEORETICAL CHEMISTRY ACCOUNTS*. ISSN 1432-881X, 2018, vol. 137, no. 11, pp., Registrované v: WOS

18. [1.1] SIVADAS, Nikhil - OKAMOTO, Satoshi - XU, Xiaodong - FENNIE, Craig J. - XIAO, Di. Stacking-Dependent Magnetism in Bilayer CrI_3 . In *NANO LETTERS*. ISSN 1530-6984, 2018, vol. 18, no. 12, pp. 7658-7664., Registrované v: WOS

19. [1.1] TAO, Jianmin - PERDEW, John P. - TANG, Hong - SHAHI, Chandra. Origin of the size-dependence of the equilibrium van der Waals binding between nanostructures. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 7, pp., Registrované v: WOS

20. [1.1] TERENTJEV, Aleksandr - CONSTANTIN, Lucian A. - PITARKE, J. M. Dispersion-corrected PBEsol exchange-correlation functional. In *PHYSICAL REVIEW B*. ISSN 2469-9950, 2018, vol. 98, no. 21, pp., Registrované v: WOS

21. [1.1] VAN TROEYE, Benoit - LHERBIER, Aurelien - CHARLIER, Jean-Christophe - GONZE, Xavier. Large phosphorene in-plane contraction induced by interlayer interactions in graphene-phosphorene heterostructures. In *PHYSICAL REVIEW*

MATERIALS. ISSN 2475-9953, 2018, vol. 2, no. 7, pp., Registrované v: WOS

22. [1.1] WANG, Na - ZHANG, Wei-bing - TANG, Bi-yu - GAO, Hai-Tao - HE, En-jie - WANG, Lei. Structural, elastic and electronic properties of typical NdMgT₄ (T = Co, Ni, Cu) alloys from ab initio calculation. In PHYSICA B-CONDENSED MATTER. ISSN 0921-4526, 2018, vol. 540, no., pp. 38-42., Registrované v: WOS

23. [1.1] YAGHOUBI, Alireza - MASENELLI-VARLOT, Karine - BOISRON, Olivier - RAMESH, S. - MELINON, Patrice. Is Graphitic Silicon Carbide (Silagraphene) Stable? In CHEMISTRY OF MATERIALS. ISSN 0897-4756, 2018, vol. 30, no. 20, pp. 7234-7244., Registrované v: WOS

24. [1.1] ZHANG, Yue-Yu - CHEN, Shiyu - XU, Peng - XIANG, Hongjun - GONG, Xin-Gao - WALSH, Aron - WEI, Su-Huai. Intrinsic Instability of the Hybrid Halide Perovskite Semiconductor CH₃NH₃PbI₃. In CHINESE PHYSICS LETTERS. ISSN 0256-307X, 2018, vol. 35, no. 3, pp., Registrované v: WOS

25. [1.1] ZHAO, Qiyi - GUO, Yaohui - ZHOU, Yixuan - YAO, Zehan - REN, Zhaoyu - BAI, Jintao - XU, Xinlong. Band alignments and heterostructures of monolayer transition metal trichalcogenides MX₃ (M = Zr, Hf; X = S, Se) and dichalcogenides MX₂ (M = Tc, Re; X = S, Se) for solar applications. In NANOSCALE. ISSN 2040-3364, 2018, vol. 10, no. 7, pp. 3547-3555., Registrované v: WOS

26. [1.1] ZUPANIC, E. - VAN MIDDEN, H. J. P. - VAN MIDDEN, M. A. - STURM, S. - TCHERNYCHOVA, E. - POKROVSKII, V. Ya - ZYBTSEV, S. G. - NASRETDINOVA, V. F. - ZAITSEV-ZOTOV, S. - CHEN, W. T. - PAI, Woei Wu - BENNETT, J. C. - PRODAN, A. Basic and charge density wave modulated structures of NbS₃-II. In PHYSICAL REVIEW B. ISSN 2469-9950, 2018, vol. 98, no. 17, pp., Registrované v: WOS

ADCA50 BUČKO, Tomáš - HAFNER, Jürgen. The role of spatial constraints and entropy in the adsorption and transformation of hydrocarbons catalyzed by zeolites. In Journal of Catalysis, 2015, vol. 329, p. 32-48. (2014: 6.921 - IF, Q1 - JCR, 2.688 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0021-9517.

Citácie:

1. [1.1] CHEN, Lin - FALSIG, Hanne - JANSSENS, Ton V. W. - GRONBECK, Henrik. Activation of oxygen on (NH₃-Cu-NH₃)(+) in NH₃-SCR over Cu-CHA. In JOURNAL OF CATALYSIS. ISSN 0021-9517, 2018, vol. 358, no., pp. 179-186., Registrované v: WOS

2. [1.1] CHIBANI, Siwar - BADAWI, Michael - LOISEAU, Thierry - VOLKRINGER, Christophe - CANTREL, Laurent - PAUL, Jean-Francois. A DFT study of RuO₄ interactions with porous materials: metal-organic frameworks (MOFs) and zeolites. In PHYSICAL CHEMISTRY CHEMICAL PHYSICS. ISSN 1463-9076, 2018, vol. 20, no. 24, pp. 16770-16776., Registrované v: WOS

3. [1.1] DE WISPELAERE, Kristof - VANDUYFHUYS, Louis - VAN SPEYBROECK, Veronique. Entropy Contributions to Transition State Modeling. In MODELLING AND SIMULATION IN THE SCIENCE OF MICRO- AND MESO-POROUS MATERIALS, 2018, vol., no., pp. 189-228., Registrované v: WOS

4. [1.1] GRAJCIAR, Lukas - HEARD, Christopher J. - BONDARENKO, Anton A. - POLYNSKI, Mikhail V. - MEEPRASERT, Jittima - PIDKO, Evgeny A. - NACHTIGALL, Petr. Towards operando computational modeling in heterogeneous catalysis. In CHEMICAL SOCIETY REVIEWS. ISSN 0306-0012, 2018, vol. 47, no. 22, pp. 8307-8348., Registrované v: WOS

5. [1.1] LI, Guanna - LIU, Chong - ROHLING, Roderigh - HENSEN, Emiel J. M. - PIDKO, Evgeny A. Lewis Acid Catalysis by Zeolites. In MODELLING AND SIMULATION IN THE SCIENCE OF MICRO- AND MESO-POROUS MATERIALS, 2018, vol., no., pp. 229-263., Registrované v: WOS

6. [1.1] RYBICKI, Marcin - SAUER, Joachim. Ab Initio Prediction of Proton Exchange Barriers for Alkanes at Bronsted Sites of Zeolite H-MFI. In JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. ISSN 0002-7863, 2018, vol. 140, no. 51, pp. 18151-18161., Registrované v: WOS

7. [1.1] VAN DER MYNSBRUGGE, Jeroen - JANDA, Amber - LIN, Li-Chiang - VAN SPEYBROECK, Veronique - HEAD-GORDON, Martin - BELL, Alexis T. Understanding Brønsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. In CHEMPHYSICHEM. ISSN 1439-4235, 2018, vol. 19, no. 4, pp. 341-358., Registrované v: WOS

8. [1.1] YANG, Chi-Ta - JANDA, Amber - BELL, Alexis T. - LIN, Li-Chiang. Atomistic Investigations of the Effects of Si/Al Ratio and Al Distribution on the Adsorption Selectivity of n-Alkanes in Brønsted-Acid Zeolites. In JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, 2018, vol. 122, no. 17, pp. 9397-9410., Registrované v: WOS

ADCA51 BUČKO, Tomáš - TUNEGA, Daniel - ÁNGYÁN, János G. - HAFNER, Jürgen. Ab initio study of structure and interconversion of native cellulose phases. In Journal of Physical Chemistry A, 2011, vol. 115, no. 35, p. 10097-10105. (2010: 2.732 - IF, karentované - CCC). (2011 - Current Contents). ISSN 1089-5639.

Citácie:

1. [1.1] CHEN, Pan - OGAWA, Yu - NISHIYAMA, Yoshiharu - ISMAIL, Ahmed E. - MAZEAU, Karim. I alpha to I beta mechano-conversion and amorphization in native cellulose simulated by crystal bending. In CELLULOSE. ISSN 0969-0239, 2018, vol. 25, no. 8, pp. 4345-4355., Registrované v: WOS

2. [1.1] DAI, Yuehua - ZHONG, Zhisheng - GONG, Shanshan. Effect of ZnO grain boundaries on non-linearity: first-principles calculations. In MATERIALS RESEARCH EXPRESS. ISSN 2053-1591, 2018, vol. 5, no. 6, pp., Registrované v: WOS

3. [1.1] KUBICKI, James D. - YANG, Hui - SAWADA, Daisuke - O'NEILL, Hugh - OEHME, Daniel - COSGROVE, Daniel. The Shape of Native Plant Cellulose Microfibrils. In SCIENTIFIC REPORTS. ISSN 2045-2322, 2018, vol. 8, no., pp., Registrované v: WOS

4. [1.1] LOUSADA, Claudio M. - SOPHONRAT, Nanta - YANG, Weihong. Mechanisms of Formation of H₂, HO₂, and Water and of Water Desorption in the Early Stages of Cellulose Pyrolysis. In JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, 2018, vol. 122, no. 23, pp. 12168-12176., Registrované v: WOS

5. [1.1] OEHME, Daniel P. - YANG, Hui - KUBICKI, James D. An evaluation of the structures of cellulose generated by the CHARMM force field: comparisons to in planta cellulose. In CELLULOSE. ISSN 0969-0239, 2018, vol. 25, no. 7, pp. 3755-3777., Registrované v: WOS

ADCA52 BÜHL, Michael - KAUPP, Martin - MALKINA, Olga - MALKIN, Vladimír. The DFT route to NMR

chemical shifts. In *Journal of Computational Chemistry*, 1999, vol. 20, no. 1, p. 91-105. (1998: 2.860 - IF, karentované - CCC). (1999 - Current Contents). ISSN 0192-8651.

Citácie:

1. [1.1] ANTUSEK, Andrej - REPISKY, Michal - JASZUNSKI, Michal - JACKOWSKI, Karol - MAKULSKI, Włodzimierz - MISIAK, Maria. Nuclear magnetic dipole moment of Bi-209 from NMR experiments. In *PHYSICAL REVIEW A*. ISSN 2469-9926, 2018, vol. 98, no. 5, pp., Registrované v: WOS
2. [1.1] HASLAK, Zeynep Pinar - BOZKURT, Esra - DUTAGACI, Bercem - DE PROFT, Frank - AVIYENTE, Viktorya - DE VLEESCHOUWER, Freija. A DFT approach to discriminate the antagonist and partial agonist activity of ligands binding to the NMDA receptor. In *MOLECULAR PHYSICS*. ISSN 0026-8976, 2018, vol. 116, no. 3, pp. 323-337., Registrované v: WOS
3. [1.1] KOECHER, S. S. - SCHLEKER, P. P. M. - GRAF, M. F. - EICHEL, R.A. - REUTER, K. - GRANWEHR, J. - SCHEURER, Ch. Chemical shift reference scale for Li solid state NMR derived by first-principles DFT calculations. In *JOURNAL OF MAGNETIC RESONANCE*. ISSN 1090-7807, 2018, vol. 297, no., pp. 33-41., Registrované v: WOS
4. [1.1] LINO, Jessica B. dos R. - RAMALHO, Teodorico C. Quantum Information and Nuclear Magnetic Resonance Parameters. In *REVISTA VIRTUAL DE QUIMICA*. ISSN 1984-6835, 2018, vol. 10, no. 4, pp. 940-962., Registrované v: WOS
5. [1.1] OEHME, Daniel P. - YANG, Hui - KUBICKI, James D. An evaluation of the structures of cellulose generated by the CHARMM force field: comparisons to in planta cellulose. In *CELLULOSE*. ISSN 0969-0239, 2018, vol. 25, no. 7, pp. 3755-3777., Registrované v: WOS
6. [1.1] REITER, Kevin - MACK, Fabian - WEIGEND, Florian. Calculation of Magnetic Shielding Constants with meta-GGA Functionals Employing the Multipole-Accelerated Resolution of the Identity: Implementation and Assessment of Accuracy and Efficiency. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 1, pp. 191-197., Registrované v: WOS
7. [1.1] YANG, Hui - WANG, Tuo - OEHME, Daniel - PETRIDIS, Loukas - HONG, Mei - KUBICKI, James D. Structural factors affecting C-13 NMR chemical shifts of cellulose: a computational study. In *CELLULOSE*. ISSN 0969-0239, 2018, vol. 25, no. 1, pp. 23-36., Registrované v: WOS

ADCA53 BÜCHEL, Gabriel E. - KOSSATZ, Susanne - SADIQUE, Ahmad - RAPTA, Peter - ZALIBERA, Michal - BUČINSKÝ, Lukáš - KOMOROVSKÝ, Stanislav - TELSER, Joshua - EPPINGER, Jörg - REINER, Thomas - ARION, Vladimír. cis-Tetrachlorido-bis(indazole)osmium(IV) and its osmium(III) analogues: paving the way towards the cis-isomer of the ruthenium anticancer drugs KP1019 and/or NKP1339. In *Dalton Transactions*, 2017, vol. 46, no. 35, p. 11925-11941. (2016: 4.029 - IF, Q1 - JCR, 1.229 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 1477-9226.

Citácie:

1. [1.1] DONG, Jinyun - ZHANG, Qijing - WANG, Zengtao - HUANG, Guang - LI, Shaoshun. Recent Advances in the Development of Indazole-based Anticancer Agents. In *CHEMMEDCHEM*. ISSN 1860-7179, 2018, vol. 13, no. 15, pp. 1490-1507., Registrované v: WOS
2. [1.1] GATTI, Anna - HABTEMARIAM, Abraha - ROMERO-CANELON, Isolda - SONG, Ji-Inn - HEER, Bindy - CLARKSON, Guy J. - ROGOLINO, Dominga - SADLER, Peter J. - CARCELLI, Mauro. Half-Sandwich Arene Ruthenium(II) and Osmium(II) Thiosemicarbazone Complexes: Solution Behavior and Antiproliferative Activity. In *ORGANOMETALLICS*. ISSN 0276-7333, 2018, vol. 37, no. 6, pp. 891-899., Registrované v: WOS
3. [1.1] KONKANKIT, Chiraluck C. - MARKER, Sierra C. - KNOPF, Kevin M. - WILSON, Justin J. Anticancer activity of complexes of the third row transition metals, rhenium, osmium, and iridium. In *DALTON TRANSACTIONS*. ISSN 1477-9226, 2018, vol. 47, no. 30, pp. 9934-9974., Registrované v: WOS

ADCA54 BUJDÁK, Juraj - MARTÍNEZ-MARTÍNEZ, Virginia - ARBELOA, Fernando López - IYI, Nobuo. Spectral properties of rhodamine 3B adsorbed on the surface of montmorillonites with variable layer charge. In *Langmuir*, 2007, vol. 23, no. 4, p. 1851-1859. ISSN 0743-7463.

Citácie:

1. [1.1] DING, Fan - GAO, Manglai - WANG, Jie - SHEN, Tao - ZANG, Weili. Tuning wettability by controlling the layer charge and structure of organo-vermiculites. In *JOURNAL OF INDUSTRIAL AND ENGINEERING CHEMISTRY*. ISSN 1226-086X, 2018, vol. 57, no., pp. 304-312., Registrované v: WOS
2. [1.1] KAWAMATA, Jun - SUZUKI, Yasutaka - TOMINAGA, Makoto. From adsorbed dyes to optical materials. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9*. ISSN 1572-4352, 2018, vol. 9, no., pp. 361-375., Registrované v: WOS

ADCA55 BUJDÁK, Juraj. Hybrid systems based on organic dyes and clay minerals: Fundamentals and potential applications. In *Clay Minerals*, 2015, vol. 50, no. 5, p. 549-571. (2014: 0.969 - IF, Q3 - JCR, 0.412 - SJR, Q3 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0009-8558.

Citácie:

1. [1.1] GRADOVA, Margarita A. - OSTASHEVSKAYA, Irina I. - GRADOV, Oleg V. - LOBANOV, Anton V. - IVANOV, Viktor B. Photophysical Properties and Photochemical Activity of Metal Phthalocyanines Adsorbed on Modified Montmorillonite. In *MACROHETEROCYCLES*. ISSN 1998-9539, 2018, vol. 11, no. 4, pp. 404-411., Registrované v: WOS
2. [1.1] SANO, Keito - SONOTANI, Amane - TATSUMI, Daichi - OHTANI, Yuta - SHIMADA, Tetsuya - TAKAGI, Shinsuke. Characterization of dispersed titania nanosheet under aqueous conditions and its complex formation behavior with cationic porphyrin. In *JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY*. ISSN 1010-6030, 2018, vol. 353, no., pp. 597-601., Registrované v: WOS
3. [1.1] TABACCHI, Gloria. Supramolecular Organization in Confined Nanospaces. In *CHEMPHYSICHEM*. ISSN 1439-4235, 2018, vol. 19, no. 11, pp. 1249-1297., Registrované v: WOS

ADCA56 BUJDÁK, Juraj - IYI, Nobuo. Optical properties of molecular aggregates of oxazine dyes in dispersions of clay minerals. In *Colloid and Polymer Science*, 2009, vol. 287, no. 2, p. 157-165. (2008: 1.736 - IF, karentované - CCC). (2009 - Current Contents). ISSN 0303-402X.

Citácie:

1. [1.1] GUPTA, Shipra - ZHAO, Yaopeng - VARADHARAJAN, Ramkumar - RAMAMURTHY, V. Competitive Binding of Organic Dyes between Cucurbiturils and Octa Acid. In ACS OMEGA. ISSN 2470-1343, 2018, vol. 3, no. 5, pp. 5083-5091., Registrované v: WOS

ADCA57 BUJDÁK, Juraj - RODE, B.M. The effect of smectite composition on the catalysis of peptide bond formation. In Journal of Molecular Evolution, 1996, vol. 43, no. 4, p. 326-333. ISSN 0022-2844.

Citácie:

1. [1.1] FABBIANI, Marco - PAZZI, Marco - VINCENTI, Marco - TABACCHI, Gloria - FOIS, Ettore - MARTRA, Gianmario. Does the Abiotic Formation of Oligopeptides on TiO₂ Nanoparticles Require Special Catalytic Sites? Apparently Not. In JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY. ISSN 1533-4880, 2018, vol. 18, no. 8, pp. 5854-5857., Registrované v: WOS

2. [1.1] WHICHER, Alexandra - CAMPRUBI, Eloi - PINNA, Silvana - HERSCHY, Barry - LANE, Nick. Acetyl Phosphate as a Primordial Energy Currency at the Origin of Life. In ORIGINS OF LIFE AND EVOLUTION OF BIOSPHERES. ISSN 0169-6149, 2018, vol. 48, no. 2, pp. 159-179., Registrované v: WOS

3. [1.1] ZOPE, Indraneel Suhas. Thermo-oxidative Decomposition Behavior of Polyamide 6 Nanocomposites with Structurally Different Clays. In FIRE RETARDANCY BEHAVIOR OF POLYMER/CLAY NANOCOMPOSITES. ISSN 2190-5053, 2018, vol., no., pp. 111-138., Registrované v: WOS

ADCA58 BUJDÁK, Juraj - RODE, B.M. Silica, alumina, and clay-catalyzed alanine peptide bond formation. In Journal of Molecular Evolution, 1997, vol. 45, no. 5, p. 457-466. (1996: 3.052 - IF). ISSN 0022-2844.

Citácie:

1. [1.1] FABBIANI, Marco - PAZZI, Marco - VINCENTI, Marco - TABACCHI, Gloria - FOIS, Ettore - MARTRA, Gianmario. Does the Abiotic Formation of Oligopeptides on TiO₂ Nanoparticles Require Special Catalytic Sites? Apparently Not. In JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY. ISSN 1533-4880, 2018, vol. 18, no. 8, pp. 5854-5857., Registrované v: WOS

2. [1.1] GREGOIRE, Brian - GREENWELL, H. Christopher - FRASER, Donald G. Peptide Formation on Layered Mineral Surfaces: The Key Role of Brucite-like Minerals on the Enhanced Formation of Alanine Dipeptides. In ACS EARTH AND SPACE CHEMISTRY. ISSN 2472-3452, 2018, vol. 2, no. 8, pp. 852-862., Registrované v: WOS

3. [1.1] PANTALEONE, Stefano - UGLIENGO, Piero - SODUPE, Mariona - RIMOLA, Albert. When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO₂ (101) Anatase Surface through Periodic DFT-D2 Simulations. In CHEMISTRY-A EUROPEAN JOURNAL. ISSN 0947-6539, 2018, vol. 24, no. 61, pp. 16292-16301., Registrované v: WOS

ADCA59 BUJDÁK, Juraj - RODE, B.M. Glycine oligomerization on silica and alumina. In Reaction Kinetics and Catalysis Letters, 1997, vol. 62, no. 2, p. 281-286. ISSN 0133-1736.

Citácie:

1. [1.1] PANTALEONE, Stefano - UGLIENGO, Piero - SODUPE, Mariona - RIMOLA, Albert. When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO₂ (101) Anatase Surface through Periodic DFT-D2 Simulations. In CHEMISTRY-A EUROPEAN JOURNAL. ISSN 0947-6539, 2018, vol. 24, no. 61, pp. 16292-16301., Registrované v: WOS

ADCA60 BUJDÁK, Juraj - KOMADEL, Peter. Interaction of methylene blue with reduced charge montmorillonite. In Journal of Physical Chemistry B, 1997, vol. 101, no. 44, p. 9065-9068. ISSN 1520-6106.

Citácie:

1. [1.1] ALBADARIN, Ahmad B. - SOLOMON, Samuel - ABOU DAHER, Mohamad - WALKER, Gavin. Efficient removal of anionic and cationic dyes from aqueous systems using spent Yerba Mate "Ilex paraguariensis". In JOURNAL OF THE TAIWAN INSTITUTE OF CHEMICAL ENGINEERS. ISSN 1876-1070, 2018, vol. 82, no., pp. 144-155., Registrované v: WOS

2. [1.1] KAWAMATA, Jun - SUZUKI, Yasutaka - TOMINAGA, Makoto. From adsorbed dyes to optical materials. In SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 361-375., Registrované v: WOS

3. [1.1] LAMBERT, Jean-Francois. Organic pollutant adsorption on clay minerals. In SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 195-253., Registrované v: WOS

4. [1.1] NAKATO, Teruyuki - KAWAMATA, Jun - TAKAGI, Shinsuke. Materials Chemistry of Inorganic Nanosheets-Overview and History. In INORGANIC NANOSHEETS AND NANOSHEET-BASED MATERIALS: FUNDAMENTALS AND APPLICATIONS OF TWO-DIMENSIONAL SYSTEMS, 2017, vol., no., pp. 3-31., Registrované v: WOS

5. [1.1] NAKAYAMA, Ayumi - MIZUNO, Junya - OHTANI, Yuta - SHIMADA, Tetsuya - TAKAGI, Shinsuke. Elucidation of the Adsorption Distribution of Cationic Porphyrin on the Inorganic Surface by Energy Transfer as a Molecular Ruler. In JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, 2018, vol. 122, no. 8, pp. 4365-4371., Registrované v: WOS

6. [1.1] TAGUCHI, Taiga - KOHNO, Yoshiumi - SHIBATA, Masashi - TOMITA, Yasumasa - FUKUHARA, Choji - MAEDA, Yasuhisa. An easy and effective method for the intercalation of hydrophobic natural dye into organo-montmorillonite for improved photostability. In JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS. ISSN 0022-3697, 2018, vol. 116, no., pp. 168-173., Registrované v: WOS

7. [1.1] TSUKAMOTO, Takamasa - SHIMADA, Tetsuya - TAKAGI, Shinsuke. Artificial Photosynthesis Model: Photochemical Reaction System with Efficient Light-Harvesting Function on Inorganic Nanosheets. In ACS OMEGA. ISSN 2470-1343, 2018, vol. 3, no. 12, pp. 18563-18571., Registrované v: WOS

ADCA61 BUJDÁK, Juraj - JANEK, Marián - MADEJOVÁ, Jana - KOMADEL, Peter. Influence of the layer charge density of smectites on the interaction with methylene blue. In Journal of the Chemical Society-Faraday Transactions, 1998, vol. 94, no. 23, p. 3487-3492.

Citácie:

1. [1.1] AKTER, Tahmina - SAUPE, Geoffrey B. Exceptional Sensitizer Dye Loading via a New Porous Titanium-Niobium Metal Oxide with Tris(2,2'-bipyridyl)ruthenium(II) in the Structure. In ACS APPLIED NANO MATERIALS. ISSN 2574-0970, 2018, vol. 1, no. 10, pp. 5620-5630., Registrované v: WOS

2. [1.1] KAWAMATA, Jun - SUZUKI, Yasutaka - TOMINAGA, Makoto. From adsorbed dyes to optical materials. In SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 361-375., Registrované v: WOS

WOS

3. [1.1] KIM, Aran - RYU, Seung-Jin - LEE, Jihye - JUNG, Hyun. Development of Latent Fingerprints on Nonporous and Semiporous Substrates Using Photoluminescent Eu(Phen)(2) Complex Intercalated Clay Hybrids with Enhanced Adhesion. In *JOURNAL OF FORENSIC SCIENCES*. ISSN 0022-1198, 2018, vol. 63, no. 6, pp. 1718-1726., Registrované v: WOS

ADCA62 BUJDÁK, Juraj - IYI, Nobuo - KANEKO, Yoshiro - CZÍMEROVÁ, Adriana - SASAI, Ryo. Molecular arrangement of rhodamine 6G cations in the films of layered silicates: the effect of the layer charge. In *Physical Chemistry Chemical Physics*, 2003, vol. 5, no. 20, p. 4680-4685. ISSN 1463-9076.

Citácie:

1. [1.1] NAKAYAMA, Ayumi - MIZUNO, Junya - OHTANI, Yuta - SHIMADA, Tetsuya - TAKAGI, Shinsuke. Elucidation of the Adsorption Distribution of Cationic Porphyrin on the Inorganic Surface by Energy Transfer as a Molecular Ruler. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 8, pp. 4365-4371., Registrované v: WOS

2. [1.1] SCHOONHEYDT, Robert A. - UMEMURA, Yasushi. Clay Minerals as Natural Nanosheets. In *INORGANIC NANOSHEETS AND NANOSHEET-BASED MATERIALS: FUNDAMENTALS AND APPLICATIONS OF TWO-DIMENSIONAL SYSTEMS*, 2017, vol., no., pp. 33-53., Registrované v: WOS

ADCA63 BUJDÁK, Juraj - RODE, B.M. Alumina catalyzed reactions of amino acids. In *Journal of Thermal Analysis and Calorimetry*, 2003, vol. 73, no. 3, p. 797-805. ISSN 1388-6150.

Citácie:

1. [1.1] PANTALEONE, Stefano - UGLIENGO, Piero - SODUPE, Mariona - RIMOLA, Albert. When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO₂ (101) Anatase Surface through Periodic DFT-D2 Simulations. In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 61, pp. 16292-16301., Registrované v: WOS

ADCA64 BUJDÁK, Juraj - RODE, B.M. Peptide bond formation on the surface of activated alumina: peptide chain elongation. In *Catalysis Letters*, 2003, vol. 91, no. 3-4, p. 149-154. ISSN 1011-372X.

Citácie:

1. [1.1] PANTALEONE, Stefano - UGLIENGO, Piero - SODUPE, Mariona - RIMOLA, Albert. When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO₂ (101) Anatase Surface through Periodic DFT-D2 Simulations. In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 61, pp. 16292-16301., Registrované v: WOS

ADCA65 BUJDÁK, Juraj - IYI, Nobuo. Molecular orientation of rhodamine dyes on surfaces of layered silicates. In *Journal of Physical Chemistry B*, 2005, vol. 109, no. 10, p. 4608-4615. (2005 - Current Contents, SCOPUS). ISSN 1520-6106.

Citácie:

1. [1.1] BANIK, Soma - HUSSAIN, S. A. - BHATTACHARJEE, D. Modified aggregation pattern of cresyl violet acetate adsorbed on nano clay mineral layers in Langmuir Blodgett film. In *JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY*. ISSN 1010-6030, 2018, vol. 353, no., pp. 570-580., Registrované v: WOS

2. [1.1] KAWAMATA, Jun - SUZUKI, Yasutaka - TOMINAGA, Makoto. From adsorbed dyes to optical materials. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS*, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 361-375., Registrované v: WOS

3. [1.1] MAHMOODI, A. - EBRAHIMI, M. Role of a hybrid dye-clay nano-pigment (DCNP) on corrosion resistance of epoxy coatings. In *PROGRESS IN ORGANIC COATINGS*. ISSN 0300-9440, 2018, vol. 114, no., pp. 223-232., Registrované v: WOS

4. [1.1] MARK, Michael F. - KRYMAN, Mark W. - DETTY, Michael R. - MCCAMANT, David W. Intermolecular Charge Separation in Aggregated Rhodamine Dyes Used in Solar Hydrogen Production. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 29, pp. 16519-16531., Registrované v: WOS

ADCA66 BUJDÁK, Juraj. Effect of the layer charge of clay minerals on optical properties of organic dyes. A review. In *Applied Clay Science*, 2006, vol. 34, no. 1-4, p. 58-73. (2005: 1.324 - IF, karentované - CCC). (2006 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] FUJIMURA, Takuya - SHIMADA, Tetsuya - SASAI, Ryo - TAKAGI, Shinsuke. Optical Humidity Sensing Using Transparent Hybrid Film Composed of Cationic Magnesium Porphyrin and Clay Mineral. In *LANGMUIR*. ISSN 0743-7463, 2018, vol. 34, no. 12, pp. 3572-3577., Registrované v: WOS

2. [1.1] GUPTA, Shipra - ZHAO, Yaopeng - VARADHARAJAN, Ramkumar - RAMAMURTHY, V. Competitive Binding of Organic Dyes between Cucurbiturils and Octa Acid. In *ACS OMEGA*. ISSN 2470-1343, 2018, vol. 3, no. 5, pp. 5083-5091., Registrované v: WOS

3. [1.1] ISHIDA, Yohei - TAKAGI, Shinsuke. Photoenergy Conversion. In *INORGANIC NANOSHEETS AND NANOSHEET-BASED MATERIALS: FUNDAMENTALS AND APPLICATIONS OF TWO-DIMENSIONAL SYSTEMS*, 2017, vol., no., pp. 357-371., Registrované v: WOS

4. [1.1] KAWAMATA, Jun - SUZUKI, Yasutaka - TOMINAGA, Makoto. From adsorbed dyes to optical materials. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS*, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 361-375., Registrované v: WOS

5. [1.1] LIVANI, Milad Jamal - GHORBANI, Mohsen. Fabrication of NiFe₂O₄ magnetic nanoparticles loaded on activated carbon as novel nanoadsorbent for Direct Red 31 and Direct Blue 78 adsorption. In *ENVIRONMENTAL TECHNOLOGY*. ISSN 0959-3330, 2018, vol. 39, no. 23, pp. 2977-2993., Registrované v: WOS

6. [1.1] NAKAYAMA, Ayumi - MIZUNO, Junya - OHTANI, Yuta - SHIMADA, Tetsuya - TAKAGI, Shinsuke. Elucidation of the Adsorption Distribution of Cationic Porphyrin on the Inorganic Surface by Energy Transfer as a Molecular Ruler. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 8, pp. 4365-4371., Registrované v: WOS

7. [1.1] SUZUKI, Shunpei - TATSUMI, Daichi - TSUKAMOTO, Takamasa - HONNA, Ryou - SHIMADA, Tetsuya - INOUE, Haruo - TAKAGI, Shinsuke. Active species transfer-type artificial light harvesting system in the nanosheet Dye complexes: Utilization of longer wavelength region of sunlight. In *TETRAHEDRON LETTERS*. ISSN 0040-4039, 2018, vol. 59, no. 6, pp. 528-531., Registrované v: WOS

8. [1.1] TSUKAMOTO, Takamasa - SHIMADA, Tetsuya - TAKAGI, Shinsuke. Artificial Photosynthesis Model: Photochemical

Reaction System with Efficient Light-Harvesting Function on Inorganic Nanosheets. In ACS OMEGA. ISSN 2470-1343, 2018, vol. 3, no. 12, pp. 18563-18571., Registrované v: WOS

- ADCA67 BUJDÁK, Juraj - IYI, Nobuo. Molecular aggregation of rhodamine dyes in dispersions of layered silicates: Influence of dye molecular structure and silicate properties. In Journal of Physical Chemistry B, 2006, vol. 110, no. 5, p. 2180-2186. (2005: 4.033 - IF, karentované - CCC). (2006 - Current Contents, WOS, SCOPUS). ISSN 1520-6106.

Citácie:

1. [1.1] KONG, Di - LIU, Yunfang - LI, Yangyang - CHI, Weidong - HUANG, Qigu - YU, Changyuan. Facile preparation and dye removal properties of Fe₃O₄@carbon nanocomposite. In MICRO & NANO LETTERS. ISSN 1750-0443, 2018, vol. 13, no. 2, pp. 219-222., Registrované v: WOS
2. [1.1] LIN, Shu-Yi - WANG, Meng-Ren - CHIU, Shih-Jiuan - LIN, Chien-Yu - HU, Teh-Min. S-Nitrosothiols (SNO) as light-responsive molecular activators for post-synthesis fluorescence augmentation in fluorophore-loaded nanospheres. In JOURNAL OF MATERIALS CHEMISTRY B. ISSN 2050-750X, 2018, vol. 6, no. 1, pp. 153-164., Registrované v: WOS
3. [1.1] TEEPAKAKORN, Aranee Pleng - BUREEKAEW, Sareeya - OGAWA, Makoto. Adsorption-Induced Dye Stability of Cationic Dyes on Clay Nanosheets. In LANGMUIR. ISSN 0743-7463, 2018, vol. 34, no. 46, pp. 14069-14075., Registrované v: WOS

- ADCA68 BUJDÁK, Juraj - IYI, Nobuo - SASAI, Ryo. Spectral properties, formation of dye molecular aggregates, and reactions in rhodamine 6G/layered silicate dispersions. In Journal of physical chemistry. B.Materials, surfaces, interfaces, and biophysical, 2004, vol. 108, no. 14, p. 4470-4477. ISSN 1520-6106.

Citácie:

1. [1.1] BANIK, Soma - HUSSAIN, S. A. - BHATTACHARJEE, D. Modified aggregation pattern of cresyl violet acetate adsorbed on nano clay mineral layers in Langmuir Blodgett film. In JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY. ISSN 1010-6030, 2018, vol. 353, no., pp. 570-580., Registrované v: WOS

- ADCA69 BUJDÁK, Juraj - IYI, Nobuo. Spectral and structural characteristics of oxazine 4/hexadecyltrimethylammonium montmorillonite films. In Chemistry of Materials, 2006, vol. 18, no. 10, p. 2618-2624. ISSN 0897-4756.

Citácie:

1. [1.1] BANIK, Soma - HUSSAIN, S. A. - BHATTACHARJEE, D. Modified aggregation pattern of cresyl violet acetate adsorbed on nano clay mineral layers in Langmuir Blodgett film. In JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY. ISSN 1010-6030, 2018, vol. 353, no., pp. 570-580., Registrované v: WOS

- ADCA70 BUJDÁK, Juraj. Effect of layer charge on the formation of polymer/layered silicate nanocomposites: Intercalation of polystyrene. In Journal of Physical Chemistry C, 2015, vol. 119, no. 21, p. 12016-12022. (2014: 4.772 - IF, Q1 - JCR, 2.027 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 1932-7447.

Citácie:

1. [1.1] DA SILVA TORIN, Rondes Ferreira - CAMANI, Paulo Henrique - DA SILVA, Larissa Nunes - PEREIRA SATO, Juliana Alves - FERREIRA, Fabio Furlan - ROSA, Derval dos Santos. Effect of clay and clay/essential oil in packaging films. In POLYMER COMPOSITES. ISSN 0272-8397, 2018, vol. 39, no. 11, pp. 4034-4040., Registrované v: WOS
2. [1.1] ZHULINA, E. B. - LEERMAKERS, F. A. M. - BORISOV, O. Effect of chain architecture on properties of self-assembled dendron brushes. In POLYMER. ISSN 0032-3861, 2018, vol. 144, no., pp. 142-149., Registrované v: WOS

- ADCA71 BUJDÁK, Juraj. Layer-by-layer assemblies composed of polycationic electrolyte, organic dyes, and layered silicates. In Journal of Physical Chemistry C, 2014, vol. 118, no. 13, p. 7152-7162. (2013: 4.835 - IF, 2.134 - SJR, karentované - CCC). (2014 - Current Contents, WOS, SCOPUS). ISSN 1932-7447.

Citácie:

1. [1.1] BRICKS, Julia L. - SLOMINSKII, Yuri L. - PANAS, Ihor D. - DEMCHENKO, Alexander P. Fluorescent J-aggregates of cyanine dyes: basic research and applications review. In METHODS AND APPLICATIONS IN FLUORESCENCE. ISSN 2050-6120, 2018, vol. 6, no. 1, pp., Registrované v: WOS
2. [1.1] HANSDA, Chaitali - MAITI, Pradip - SINGHA, Tanmoy - PAL, Manisha - HUSSAIN, Syed Arshad - PAUL, Sharmistha - PAUL, Pabitra Kumar. Photophysical study of the interaction between ZnO nanoparticles and globular protein bovine serum albumin in solution and in a layer-by-layer self-assembled film. In JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS. ISSN 0022-3697, 2018, vol. 121, no., pp. 110-120., Registrované v: WOS
3. [1.1] MATEJDES, Marian - HIMENO, Daisuke - SUZUKI, Yasutaka - KAWAMATA, Jun. The effect of the negative charge density on switchable properties of pseudoisocyanine dye. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2017, vol. 144, no., pp. 54-59., Registrované v: WOS

- ADCA72 BUJDÁK, Juraj - CZÍMEROVÁ, Adriana - ARBELOA, Fernando López. Two-step resonance energy transfer between dyes in layered silicate films. In Journal of Colloid and Interface Science, 2011, vol. 364, no. 2, p. 497-504. (2010: 3.066 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0021-9797.

Citácie:

1. [1.1] DIAS, Guilherme - PRADO, Manoela - LIGABUE, Rosane - POIRIER, Mathilde - LE ROUX, Christophe - MARTIN, Francois - FERY-FORGUES, Suzanne - EINLOFT, Sandra. Synthetic talc as a new platform for producing fluorescent clay polyurethane nanocomposites. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 158, no., pp. 37-45., Registrované v: WOS
2. [1.1] UMEMURA, Yasushi. Preparation and application of clay mineral films. In SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 377-396., Registrované v: WOS

- ADCA73 BUJDÁK, Juraj - HACKETT, E. - GIANNELIS, E.P. Effect of layer charge on the intercalation of

poly(ethylene oxide) in layered silicates: Implications on nanocomposite polymer electrolytes. In *Chemistry of Materials*, 2000, vol. 12, no. 8, p. 2168-2174.

Citácie:

1. [1.1] GEORGE, Jeffrey - ISHIDA, Hatsuo. A review on the very high nanofiller-content nanocomposites: Their preparation methods and properties with high aspect ratio fillers. In *PROGRESS IN POLYMER SCIENCE*. ISSN 0079-6700, 2018, vol. 86, no., pp. 1-39., Registrované v: WOS

2. [1.1] ZHANG, Guangjian - WANG, Jincheng. Preparation of novel flame-retardant organoclay and its application to natural rubber composites. In *JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS*. ISSN 0022-3697, 2018, vol. 115, no., pp. 137-147., Registrované v: WOS

ADCA74 BUJDÁK, Juraj - JANEK, Marián - MADEJOVÁ, Jana - KOMADEL, Peter. Methylene blue interactions with reduced-charge smectites. In *Clays and Clay Minerals*, 2001, vol. 49, no. 3, p. 244-254. (2001 - Current Contents). ISSN 0009-8604.

Citácie:

1. [1.1] NARVEKAR, Apurva A. - FERNANDES, J. B. - TILVE, S. G. Adsorption behavior of methylene blue on glycerol based carbon materials. In *JOURNAL OF ENVIRONMENTAL CHEMICAL ENGINEERING*. ISSN 2213-2929, 2018, vol. 6, no. 2, pp. 1714-1725., Registrované v: WOS

2. [1.1] SMYNTYNA, V. - SKOBEEVA, V. Heterogeneous Systems with Ag Nanoparticles. In *NANOSTRUCTURED MATERIALS FOR THE DETECTION OF CBRN*. ISSN 1874-6489, 2018, vol., no., pp. 301-308., Registrované v: WOS

ADCA75 BUJDÁK, Juraj - CZÍMEROVÁ, Adriana - IYI, Nobuo. Structure of cationic dyes assemblies intercalated in the films of montmorillonite. In *Thin Solid Films*, 2008, vol. 517, no. 2, p. 793-799. (2007: 1.690 - IF). ISSN 0040-6090.

Citácie:

1. [1.1] KANG, Shichang - ZHAO, Yunliang - WANG, Wei - ZHANG, Tingting - CHEN, Tianxing - YI, Hao - RAO, Feng - SONG, Shaoxian. Removal of methylene blue from water with montmorillonite nanosheets/chitosan hydrogels as adsorbent. In *APPLIED SURFACE SCIENCE*. ISSN 0169-4332, 2018, vol. 448, no., pp. 203-211., Registrované v: WOS

ADCA76 BUJDÁK, Juraj - IYI, Nobuo. Spectral properties and structure of the J-aggregates of pseudoisocyanine dye in layered silicate films. In *Journal of Colloid and Interface Science*, 2008, vol. 326, no. 2, p. 426-432. (2007: 2.309 - IF). ISSN 0021-9797.

Citácie:

1. [1.1] BRICKS, Julia L. - SLOMINSKII, Yuri L. - PANAS, Ihor D. - DEMCHENKO, Alexander P. Fluorescent J-aggregates of cyanine dyes: basic research and applications review. In *METHODS AND APPLICATIONS IN FLUORESCENCE*. ISSN 2050-6120, 2018, vol. 6, no. 1, pp., Registrované v: WOS

ADCA77 BUJDÁK, Juraj - IYI, Nobuo - FUJITA, Taketoshi. The aggregation of methylene blue in montmorillonite dispersions. In *Clay Minerals*, 2002, vol. 37, no. 1, p. 121-133. (2001: 0.610 - IF, karentované - CCC). (2002 - Current Contents). ISSN 0009-8558.

Citácie:

1. [1.1] NAKATO, Teruyuki - KAWAMATA, Jun - TAKAGI, Shinsuke. Materials Chemistry of Inorganic Nanosheets-Overview and History. In *INORGANIC NANOSHEETS AND NANOSHEET-BASED MATERIALS: FUNDAMENTALS AND APPLICATIONS OF TWO-DIMENSIONAL SYSTEMS*, 2017, vol., no., pp. 3-31., Registrované v: WOS

2. [1.1] SADRI, Shahrzad - JOHNSON, Bruce B. - RUYTER-HOOLEY, Maika - ANGOVE, Michael J. The adsorption of norriptyline on montmorillonite, kaolinite and gibbsite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 165, no., pp. 64-70., Registrované v: WOS

ADCA78 BUJDÁK, Juraj - RODE, B.M. Preferential amino acid sequences in alumina-catalyzed peptide bond formation. In *Journal of Inorganic Biochemistry*, 2002, vol. 90, no. 1-2, p. 1-7.

Citácie:

1. [1.1] PANTALEONE, Stefano - UGLIENGO, Piero - SODUPE, Mariona - RIMOLA, Albert. When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO₂ (101) Anatase Surface through Periodic DFT-D2 Simulations. In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 61, pp. 16292-16301., Registrované v: WOS

2. [1.1] WANG, Yanshi - WANG, Xiaoyu - LIN, Jingsheng - YAO, Bo - WANG, Guanghui - ZHAO, Yuandong - ZHANG, Xinhang - LIN, Bin - LIU, Yang - CHENG, Maosheng - LIU, Yongxiang. Ynesulfonamide-Based Silica Gel and Alumina-Mediated Diastereoselective Cascade Cyclizations to Spiro[indoline-3,3-pyrrolidin]-2-ones under Neat Conditions. In *ADVANCED SYNTHESIS & CATALYSIS*. ISSN 1615-4150, 2018, vol. 360, no. 7, pp. 1483-1492., Registrované v: WOS

ADCA79 BUJDÁK, Juraj - IYI, Nobuo - FUJITA, Taketoshi. Aggregation and stability of 1,1'-diethyl-4,4'-cyanine dye on the surface of layered silicates with different charge densities. In *Colloids and Surfaces : A: Physicochemical and Engineering Aspects*. - Elsevier B.V., 2002, vol. 207, no. 1-3, p. 207-214. ISSN 0927-7757.

Citácie:

1. [1.1] RIBEIRO, Halisson L. - DE OLIVEIRA, Ana Vitoria - DE BRITO, Edy S. - RIBEIRO, Paulo R. V. - SOUZA FILHO, Men de Sa M. - AZEREDO, Henriette M. C. Stabilizing effect of montmorillonite on acerola juice anthocyanins. In *FOOD CHEMISTRY*. ISSN 0308-8146, 2018, vol. 245, no., pp. 966-973., Registrované v: WOS

ADCA80 BUJDÁK, Juraj - DANKO, Martin - CHORVÁT, Dušan Jr. - CZÍMEROVÁ, Adriana - SÝKORA, J. - LANG, K. Selective modification of layered silicate nanoparticle edges with fluorophores. In *Applied Clay Science*, 2012, vol. 65-66, p. 152 - 157. (2011: 2.474 - IF, 1.165 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] MAISANABA, S. - GUZMAN-GUILLEN, R. - PUERTO, M. - GUTIERREZ-PRAENA, D. - ORTUNO, N. - JOS, A. In vitro

toxicity evaluation of new silane-modified clays and the migration extract from a derived polymer-clay nanocomposite intended to food packaging applications. In JOURNAL OF HAZARDOUS MATERIALS. ISSN 0304-3894, JAN 5 2018, vol. 341, p. 313-320., Registrované v: WOS

2. [1.1] NAKAYAMA, A. - MIZUNO, J. - OHTANI, Y. - SHIMADA, T. - TAKAGI, S. *Elucidation of the Adsorption Distribution of Cationic Porphyrin on the Inorganic Surface by Energy Transfer as a Molecular Ruler. In JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, MAR 1 2018, vol. 122, no. 8, p. 4365-4371., Registrované v: WOS*

ADCA81 BUJDAK, Juraj - RODE, B.M. The effect of clay structure on peptide bond formation catalysis. In *Journal of Molecular Catalysis A : Chemical*, 1999, vol. 144, no. 1, p. 129-136. (1998: 1.660 - IF).

Citácie:

1. [1.1] GREGOIRE, Brian - GREENWELL, H. Christopher - FRASER, Donald G. *Peptide Formation on Layered Mineral Surfaces: The Key Role of Brucite-like Minerals on the Enhanced Formation of Alanine Dipeptides. In ACS EARTH AND SPACE CHEMISTRY. ISSN 2472-3452, 2018, vol. 2, no. 8, pp. 852-862., Registrované v: WOS*

2. [1.1] ZOPE, Indraneel Suhas. *Thermo-oxidative Decomposition Behavior of Polyamide 6 Nanocomposites with Structurally Different Clays. In FIRE RETARDANCY BEHAVIOR OF POLYMER/CLAY NANOCOMPOSITES. ISSN 2190-5053, 2018, vol., no., pp. 111-138., Registrované v: WOS*

ADCA82 BUJDAK, Juraj - RODE, B.M. Silica, alumina and clay catalyzed peptide bond formation: Enhanced efficiency of alumina catalyst. In *Origins of Life and Evolution of the Biosphere*, 1999, vol. 29, no. 5, p. 451-461. (1998: 0.750 - IF).

Citácie:

1. [1.1] PANTALEONE, Stefano - UGLIENGO, Piero - SODUPE, Mariona - RIMOLA, Albert. *When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO₂ (101) Anatase Surface through Periodic DFT-D2 Simulations. In CHEMISTRY-A EUROPEAN JOURNAL. ISSN 0947-6539, 2018, vol. 24, no. 61, pp. 16292-16301., Registrované v: WOS*

ADCA83 BUJDAK, Juraj - RODE, B.M. Activated alumina as an energy source for peptide bond formation: Consequences for mineral-mediated prebiotic processes. In *Amino Acids*, 2001, vol. 21, no. 3, p. 281-291.

Citácie:

1. [1.1] MCKEE, Aaron D. - SOLANO, Martin - SAYDJARI, Andrew - BENNETT, Christopher J. - HUD, Nicholas V. - ORLANDO, Thomas M. *A Possible Path to Prebiotic Peptides Involving Silica and Hydroxy Acid-Mediated Amide Bond Formation. In CHEMBIOCHEM. ISSN 1439-4227, 2018, vol. 19, no. 18, pp. 1913-1917., Registrované v: WOS*

2. [1.1] PANTALEONE, Stefano - UGLIENGO, Piero - SODUPE, Mariona - RIMOLA, Albert. *When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO₂ (101) Anatase Surface through Periodic DFT-D2 Simulations. In CHEMISTRY-A EUROPEAN JOURNAL. ISSN 0947-6539, 2018, vol. 24, no. 61, pp. 16292-16301., Registrované v: WOS*

ADCA84 BUJDAKOVÁ, Helena - BUJDAKOVÁ, Veronika - MÁJEKOVÁ, Hyacinta - GAÁLOVÁ, Barbora - BIZOVSKÁ, Valéria - BOHÁČ, Peter - BUJDAK, Juraj. Antimicrobial activity of organoclays based on quaternary alkylammonium and alkylphosphonium surfactants and montmorillonite. In *Applied Clay Science*, 2018, vol. 158, no., p. 21-28. (2017: 3.641 - IF, Q1 - JCR, 0.992 - SJR, Q1 - SJR, karentované - CCC). (2018 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] SALES MONTEIRO, Mayra Kerolly - LEAL DE OLIVEIRA, Victor Rafael - GOMES DOS SANTOS, Francisco Klebson - DE BARROS NETO, Eduardo Lins - DE LIMA LEITE, Ricardo Henrique - MENDES AROUCHA, Edna Maria - DE OLIVEIRA SILVA, Karyn Nathallye. *Influence of the ionic and nonionic surfactants mixture in the structure and properties of the modified bentonite clay. In JOURNAL OF MOLECULAR LIQUIDS. ISSN 0167-7322, 2018, vol. 272, no., pp. 990-998., Registrované v: WOS*

ADCA85 BYSTRICKÁ, Zuzana - BYSTRICKÝ, Roman - LEHOTAY, Jozef. Thermodynamic study of HPLC enantioseparations of some sulfur-containing amino acids on teicoplanin columns in ion-pairing reversed-phase mode. In *Journal of Liquid Chromatography & Related Technologies*, 2016, vol. 30, no. 16, p. 775-781. (2015: 0.669 - IF, Q4 - JCR, 0.291 - SJR, Q2 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 1082-6076.

Citácie:

1. [1.1] GRENO, Maider - LUISA MARINA, Maria - CASTRO-PUYANA, Maria. *Effect of the combined use of gamma-cyclodextrin and a chiral ionic liquid on the enantiomeric separation of homocysteine by capillary electrophoresis. In JOURNAL OF CHROMATOGRAPHY A. ISSN 0021-9673, 2018, vol. 1568, no., pp. 222-228., Registrované v: WOS*

ADCA86 CAPEK, Peter - DRÁBIK, Milan - TURJAN, Jozef. Characterization of starch and its mono and hybrid derivatives by thermal analysis and FT-IR spectroscopy. In *Journal of Thermal Analysis and Calorimetry*, 2010, vol. 99, no. 2, p. 667-673. (2009: 1.587 - IF, karentované - CCC). (2010 - Current Contents). ISSN 1388-6150.

Citácie:

1. [1.1] ARAUJO, Antonio - GALVAO, Andressa - SILVA FILHO, Carlos - MENDES, Francisco - OLIVEIRA, Marilia - BARBOSA, Francisco - SOUSA FILHO, Men - BASTOS, Maria. *Okra mucilage and corn starch bio-based film to be applied in food. In POLYMER TESTING. ISSN 0142-9418, 2018, vol. 71, no., pp. 352-361., Registrované v: WOS*

2. [1.1] BUJDAKOVA, H. - BUJDAKOVA, V. - MAJEKOVA-KOSCOVA, H. - GAALOVA, B. - BIZOVSKA, V. - BOHAC, P. - BUJDAK, J. Antimicrobial activity of organoclays based on quaternary alkylammonium and alkylphosphonium surfactants and montmorillonite. In *APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 158, no., pp. 21-28., Registrované v: WOS*

3. [1.1] KACZMARSKA, Karolina - GRABOWSKA, Beata - SPYCHAJ, Tadeusz - ZDANOWICZ, Magdalena - SITARZ, Maciej - BOBROWSKI, Artur - CUKROWICZ, Sylwia. *Effect of microwave treatment on structure of binders based on sodium carboxymethyl starch: FT-IR, FT-Raman and XRD investigations. In SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY. ISSN 1386-1425, 2018, vol. 199, no., pp. 387-393., Registrované v: WOS*

- ADCA87 CZÍMEROVÁ, Adriana - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana - ČEKLOVSKÝ, Alexander. Unique photoactive nanocomposites based on rhodamine 6G/polymer/montmorillonite hybrid systems. In *Journal of Polymer Science. Part B. Polymer Physics*, 2013, vol. 51, no. 23, p. 1672-1679. (2012: 2.221 - IF, 1.059 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 0887-6266.(APVV-0291-11 : Fotoaktívne hybridné nanomateriály s luminiscenčnými a antimikrobiálnymi vlastnosťami. APVV-0362-10 : Organoily a ich kompozity s polymérmi).
- Citácie:
- [1.1] BUJDAK, Juraj. *Hybrids with Functional Dyes*. In *INORGANIC NANOSHEETS AND NANOSHEET-BASED MATERIALS: FUNDAMENTALS AND APPLICATIONS OF TWO-DIMENSIONAL SYSTEMS*, 2017, vol., no., pp. 419-465., Registrované v: WOS
 - [1.1] SERWICKA, Ewa M. - ZIMOWSKA, Malgorzata - DURACZYNSKA, Dorota - NAPRUSZEWSKA, Bogna D. - NATTICH-RAK, Malgorzata - MORDARSKI, Grzegorz - LITYNSKA-DOBRZYNSKA, Lidia - PALKOVA, Helena. *PDDA-Montmorillonite Composites Loaded with Ru Nanoparticles: Synthesis, Characterization, and Catalytic Properties in Hydrogenation of 2-Butanone*. In *POLYMERS*. ISSN 2073-4360, 2018, vol. 10, no. 8, pp., Registrované v: WOS
- ADCA88 CZÍMEROVÁ, Adriana - BUJDAK, Juraj - GÁPLOVSKÝ, A. The aggregation of thionine and methylene blue dye in smectite dispersion. In *Colloids and Surfaces.A: Physicochemical and Engineering Aspects*, 2004, vol. 243, no. 1-3, p. 89-96. ISSN 0927-7757.
- Citácie:
- [1.1] GILANI, A. *Ghanadzadeh* - POORMOHAMMADI-AHANDANI, Z. - KIAN, R. *Additive-induced aggregate changes of two structurally similar dyes in aqueous solutions: A comparative photophysical study*. In *SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY*. ISSN 1386-1425, 2018, vol. 189, no., pp. 543-555., Registrované v: WOS
- ADCA89 CZÍMEROVÁ, Adriana - BUJDAK, Juraj - DOHRMANN, Reiner. Traditional and novel methods for estimating the layer charge of smectites. In *Applied Clay Science*, 2006, vol. 34, no. 1-4, p. 2-13. (2005: 1.324 - IF, karentované - CCC). (2006 - Current Contents). ISSN 0169-1317.
- Citácie:
- [1.1] AYAZI, Zahra - POURVALI, Mehri - MATIN, Amir Abbas. *Preparation of a novel stir bar coating based on montmorillonite doped polypyrrole/nylon-6 nanocomposite for sorptive extraction of organophosphorous pesticides in aqueous samples*. In *INTERNATIONAL JOURNAL OF ENVIRONMENTAL ANALYTICAL CHEMISTRY*. ISSN 0306-7319, 2018, vol. 98, no. 2, pp. 138-155., Registrované v: WOS
 - [1.1] DELAVERNHE, L. - PILAVTEPE, M. - EMMERICH, K. *Cation exchange capacity of natural and synthetic hectorite*. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 151, no., pp. 175-180., Registrované v: WOS
 - [1.1] JEEVA, Mark - ZUHAIRI, Wan W. Y. *Adsorption of Acid Blue 25 Dye by Bentonite and Surfactant Modified Bentonite*. In *2017 UKM FST POSTGRADUATE COLLOQUIUM*. ISSN 0094-243X, 2018, vol. 1940, no., pp., Registrované v: WOS
 - [1.1] MARCO CHAMBI-PERALTA, Marvin - VIEIRA COELHO, Antonio Carlos - DE SOUZA CARVALHO, Flavio Machado - TOFFOLI, Samuel Marcio. *Effects of exchanged cation, acid treatment and high shear mechanical treatment on the swelling and the particle size distribution of vermiculite*. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 155, no., pp. 1-7., Registrované v: WOS
 - [1.1] MARCO-BROWN, J. L. - GUZ, L. - OLIVELLI, M. S. - SCHAMPERA, B. - TORRES SANCHEZ, R. M. - CURUTCHET, G. - CANDAL, R. *New insights on crystal violet dye adsorption on montmorillonite: Kinetics and surface complexes studies*. In *CHEMICAL ENGINEERING JOURNAL*. ISSN 1385-8947, 2018, vol. 333, no., pp. 495-504., Registrované v: WOS
 - [1.1] SHEN, Tao - GAO, Manglai - ZANG, Weili - DING, Fan - WANG, Jie. *Architecting organo silica nanosheets for regenerable cost-effective organics adsorbents*. In *CHEMICAL ENGINEERING JOURNAL*. ISSN 1385-8947, 2018, vol. 331, no., pp. 211-220., Registrované v: WOS
- ADCA90 ČÁRSKY, P. - BARTLETT, Rodney J. - FITZGERALD, G. - NOGA, Jozef - SPIRKO, V. Ab initio calculations on the energy of activation and tunneling in the automerization of cyclobutadiene. In *Journal of Chemical Physics*, 1988, vol. 89, no. 5, p. 3008-3015. ISSN 0021-9606.
- Citácie:
- [1.1] SCHOONMAKER, R. - LANCASTER, T. - CLARK, S. J. *Quantum mechanical tunneling in the automerization of cyclobutadiene*. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 10, pp., Registrované v: WOS
 - [1.1] VARRAS, Panayiotis C. - GRITZAPIS, Panagiotis S. *The transition state of the automerization reaction of cyclobutadiene: A theoretical approach using the Restricted Active Space Self Consistent Field method*. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 711, no., pp. 166-172., Registrované v: WOS
- ADCA91 ČEKLOVSKÝ, Alexander - CZÍMEROVÁ, Adriana - LANG, Kamil - BUJDAK, Juraj. Layered silicate films with photochemically active porphyrin cations. In *Pure and Applied Chemistry*, 2009, vol. 81, no. 8, p. 1385-1396. (2008: 2.237 - IF). ISSN 0033-4545.
- Citácie:
- [1.1] UMEMURA, Yasushi. *Preparation and application of clay mineral films*. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9*. ISSN 1572-4352, 2018, vol. 9, no., pp. 377-396., Registrované v: WOS
- ADCA92 ČEKLOVSKÝ, Alexander - BUJDAK, Juraj - CZÍMEROVÁ, Adriana - IYI, Nobuo. Spectral study on the molecular orientation of a tetracationic porphyrin dye on the surface of layered silicates. In *Central European Journal of Physics*, 2007, vol. 5, no. 2, p. 236-243. (2006: 0.811 - IF, karentované - CCC). (2007 - Current Contents, WOS, SCOPUS). ISSN 1895-1082.
- Citácie:
- [1.1] KAWAMATA, Jun - SUZUKI, Yasutaka - TOMINAGA, Makoto. *From adsorbed dyes to optical materials*. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9*. ISSN 1572-4352, 2018, vol. 9, no., pp. 361-375., Registrované v: WOS

- ADCA93 ČERNÁ, Andrea - CHROMČÍKOVÁ, Mária - MACHÁČEK, Jan - HRUŠKA, Branislav - LIŠKA, Marek. Viscosity and configuration entropy of glasses for CHROMPIC vitrification. In Journal of Thermal Analysis and Calorimetry, 2018, vol. 133, no. 1, p. 365-370. (2017: 2.209 - IF, Q2 - JCR, 0.587 - SJR, Q2 - SJR, karentované - CCC). (2018 - Current Contents). ISSN 1388-6150.

Citácie:

1. [1.1] GEDEON, Ondrej. Origin of glass fragility and Vogel temperature emerging from Molecular dynamics simulations. In JOURNAL OF NON-CRYSTALLINE SOLIDS. ISSN 0022-3093, 2018, vol. 498, no., pp. 109-117., Registrované v: WOS

- ADCA94 ČERNOŠEK, Zdeněk - HOLUBOVÁ, Jana - ČERNOŠKOVÁ, Eva - LIŠKA, Marek. Enthalpic relaxation and the glass transition. In Journal of Optoelectronics and Advanced Materials, 2002, vol. 4, no. 3, p. 489-503. (2001: 0.274 - IF). ISSN 1454-4164.

Citácie:

1. [1.1] KORTE, Carolin - QUODBACH, Julian. Formulation development and process analysis of drug-loaded filaments manufactured via hot-melt extrusion for 3D-printing of medicines. In PHARMACEUTICAL DEVELOPMENT AND TECHNOLOGY. ISSN 1083-7450, 2018, vol. 23, no. 10, pp. 1117-1127., Registrované v: WOS

2. [1.1] PETROVIC, Ana F. Kozmidis - STRBAC, Goran R. - STRBAC, Dragana D. Mathematical-physical imperfections in frequently used models for analyzing glass crystallization and glass transition processes. In JOURNAL OF NON-CRYSTALLINE SOLIDS. ISSN 0022-3093, 2018, vol. 502, no., pp. 89-96., Registrované v: WOS

- ADCA95 ČERNUŠÁK, Ivan - NOGA, Jozef - DIERCKSEN, G.H.F. - SADLEJ, A.J. A study of the reliability of different many-body methods: Potential energy curve for the ground state of Be₂. In Chemical Physics, 1988, vol. 125, no. 2-3, p. 255-260. ISSN 0301-0104.

Citácie:

1. [1.1] MAGOULAS, Ilias - BAUMAN, Nicholas P. - SHEN, Jun - PIECUCH, Piotr. Application of the CC(P;Q) Hierarchy of CoupledCluster Methods to the Beryllium Dimer. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 5, pp. 1350-1368., Registrované v: WOS

- ADCA96 DECARREAU, Alain - VIGIER, Nathalie - PÁLKOVÁ, Helena - PETIT, Sabine - VIEILLARD, Philippe - FONTAINE, Claude. Partitioning of lithium between smectite and solution: An experimental approach. In Geochimica et Cosmochimica Acta, 2012, vol. 85, p. 314-325. (2011: 4.259 - IF, 3.000 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 0016-7037.

Citácie:

1. [1.1] MUNK, Lee Ann - BOUTT, David F. - HYNEK, Scott A. - MORAN, Brendan J. Hydrogeochemical fluxes and processes contributing to the formation of lithium-enriched brines in a hyper-arid continental basin. In CHEMICAL GEOLOGY. ISSN 0009-2541, 2018, vol. 493, no., pp. 37-57., Registrované v: WOS

- ADCA97 DEMEL, Ondřej - KEDŽUCH, Stanislav - ŠVAŇA, Matej - TEN-NO, Seiichiro - PITTNER, Jiří - NOGA, Jozef. An explicitly correlated Mukherjee's state specific coupled cluster method: development and pilot applications. In Physical Chemistry Chemical Physics, 2012, vol. 14, p. 4753-4762. (2011: 3.573 - IF, 1.697 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 1463-9076.

Citácie:

1. [1.1] NASCIMENTO, Daniel R. - DEPRINCE, A. Eugene. Spatial and Spin Symmetry Breaking in Semidefinite-Programming-Based Hartree-Fock Theory. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 5, pp. 2418-2426., Registrované v: WOS

- ADCA98 DERKOWSKI, Arkadiusz - FRANUS, Wojciech - WANIĄK-NOWICKA, Halina - CZÍMEROVÁ, Adriana. Textural properties vs. CEC and EGME retention Na-X zeolite prepared from fly ash at room temperature. In International Journal of Mineral Processing, 2007, vol. 82, no. 2, p. 57-68. ISSN 0301-7516.

Citácie:

1. [1.1] YAO, Guangyuan - LEI, Jingjing - ZHANG, Xiaoyu - SUN, Zhiming - ZHENG, Shuilin. One-Step Hydrothermal Synthesis of Zeolite X Powder from Natural Low-Grade Diatomite. In MATERIALS. ISSN 1996-1944, 2018, vol. 11, no. 6, pp., Registrované v: WOS

- ADCA99 DERKOWSKI, Arkadiusz - FRANUS, Wojciech - BERAN, Elzbieta - CZÍMEROVÁ, Adriana. Properties and potential applications of zeolitic materials produced from fly ash using simple method of synthesis. In Powder Technology, 2006, vol. 166, no. 1, p. 47-54. ISSN 0032-5910.

Citácie:

1. [1.1] KHALID, Hammad R. - LEE, N. K. - PARK, S. M. - ABBAS, N. - LEE, H. K. Synthesis of geopolymer-supported zeolites via robust one-step method and their adsorption potential. In JOURNAL OF HAZARDOUS MATERIALS. ISSN 0304-3894, 2018, vol. 353, no., pp. 522-533., Registrované v: WOS

2. [1.1] LACH, Michal - GRELA, Agnieszka - BAJDA, Tomasz - MIERZWINSKI, Dariusz - KOMAR, Norbert - MIKULA, Janusz. Production of Zeolite Sorbents from Burning and Co-burning Biomass with Coal. In 10TH CONFERENCE ON INTERDISCIPLINARY PROBLEMS IN ENVIRONMENTAL PROTECTION AND ENGINEERING EKO-DOK 2018. ISSN 2267-1242, 2018, vol. 44, no., pp., Registrované v: WOS

3. [1.1] NIYOGI, A. - PATI, J. K. - PANIGRAHI, M. K. - PANDA, D. - CHAKARVORTY, M. - PARTHASARATHY, G. RAMAN, INFRARED, AND CHEMICAL CHARACTERIZATION OF FLY ASH-GENERATED SPHERULES. In JOURNAL OF APPLIED SPECTROSCOPY. ISSN 0021-9037, 2018, vol. 85, no. 5, pp. 856-863., Registrované v: WOS

4. [1.1] RAMIREZ-ZAMORA, R. M. - SOLIS-LOPEZ, M. - ROBLES-GUTIERREZ, I. - REYES-VIDAL, Y. - ESPEJEL-AYALA, F. A Statistical Industrial Approach for the Synthesis Conditions of Zeolites Using Fly Ash and Kaolinite. In ENVIRONMENTAL PROGRESS & SUSTAINABLE ENERGY. ISSN 1944-7442, 2018, vol. 37, no. 1, pp. 318-332., Registrované v: WOS

5. [1.1] SANCHEZ-RUIZ, A. - ROBLES-GUTIERREZ, I. - ESPEJEL-AYALA, F. PREPARATION OF ZEOLITIC MATERIAL USING NATURAL CLINOPTILOLITE FOR CO₂ CAPTURE. In REVISTA MEXICANA DE INGENIERIA QUIMICA. ISSN 1665-

2738, 2018, vol. 17, no. 2, pp. 573-585., Registrované v: WOS

6. [1.1] TAUANOV, Z. - TSAKIRIDIS, P. E. - MIKHALOVSKY, S. - INGLEZAKIS, V. J. Synthetic coal fly ash-derived zeolites doped with silver nanoparticles for mercury (II) removal from water. In JOURNAL OF ENVIRONMENTAL MANAGEMENT. ISSN 0301-4797, 2018, vol. 224, no., pp. 164-171., Registrované v: WOS

7. [1.1] TAUANOV, Zhandos - SHAH, Dhawal - INGLEZAKIS, Vassilis - JAMWAL, Prashant K. Hydrothermal synthesis of zeolite production from coal fly ash: A heuristic approach and its optimization for system identification of conversion. In JOURNAL OF CLEANER PRODUCTION. ISSN 0959-6526, 2018, vol. 182, no., pp. 616-623., Registrované v: WOS

ADCA100 DIMOS, Konstantinos - JANKOVIČ, Ľuboš - KOUTSELAS, Ioannis - KARAKASSIDES, M.A. - ZBORIL, Radek - KOMADEL, Peter. Low-temperature synthesis and characterization of gallium nitride quantum dots in ordered mesoporous silica. In Journal of Physical Chemistry C, 2012, vol. 116, no. 1, p. 1185-1194. (2011: 4.805 - IF, 2.320 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 1932-7447.

Citácie:

1. [1.1] MBAKAAN, C. - AHMEN, I. - AMAH, A. N. - ONOJAH, A. D. - KOAO, L. White-light-emitting Dy³⁺-doped amorphous SiO₂ nanophosphors derived from rice husk. In APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING. ISSN 0947-8396, 2018, vol. 124, no. 11, pp., Registrované v: WOS

ADCA101 DONAUEROVÁ, Alena - BUJDÁK, Juraj - SMOLINSKÁ, Miroslava - BUJDÁKOVÁ, Helena. Photophysical and antibacterial properties of complex systems based on smectite, a cationic surfactant and methylene blue. In Journal of Photochemistry and Photobiology : B: Biology, 2015, vol. 151, p. 135-141. (2014: 2.960 - IF, Q2 - JCR, 0.792 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 1011-1344.

Citácie:

1. [1.1] MANEEDAENG, Attaphon - PHOEMBOON, Sakonwan - CHANTHASANA, Panjamaphon - CHUDAPONGSE, Nuannoi. Synthesis, interfacial properties, and antimicrobial activity of a new cationic gemini surfactant. In KOREAN JOURNAL OF CHEMICAL ENGINEERING. ISSN 0256-1115, 2018, vol. 35, no. 11, pp. 2313-2320., Registrované v: WOS

ADCA102 DRDLÍKOVÁ, K. - KLEMENT, Róbert - DRDLÍK, Daniel - SPÚSTA, Tomáš - GALUSEK, Dušan - MACA, Karel. Luminescent Er³⁺ doped transparent alumina ceramics. In Journal of the European Ceramic Society, 2017, vol.37, no. 7, p. 2695-2703. (2016: 3.454 - IF, Q1 - JCR, 1.142 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0955-2219.

Citácie:

1. [1.1] XU, Boxu - DONG, Guangzong - LIU, Juncheng - ZOU, Kaishun - WANG, Danping. The luminescence regulation effect of Na⁺ on the Yb³⁺/Er³⁺ co-doped Y₂O₃ up-conversion films. In JOURNAL OF LUMINESCENCE. ISSN 0022-2313, 2018, vol. 203, no., pp. 16-25., Registrované v: WOS

2. [1.1] YAVETSKIY, R. P. - DOBROTVOVSKAYA, M. V. - DOROSHENKO, A. G. - TOLMACHEV, A. V. - PETRUSHA, I. A. - TURKEVICH, V. Z. - TOMALA, R. - HRENIAK, D. - STREK, W. - BAUMER, V. N. Fabrication and luminescent properties of (Y_{0.99}Eu_{0.01})(2)O₃ transparent nanostructured ceramics. In OPTICAL MATERIALS. ISSN 0925-3467, 2018, vol. 78, no., pp. 285-291., Registrované v: WOS

3. [1.1] ZHANG, Yuanyuan - LUO, Laihui - LI, Kaixuan - LI, Weiping - HOU, Yafei. Large and reversible in-situ up-conversion photoluminescence modulation based on photochromism via electric-field and thermal stimulus in ferroelectrics. In JOURNAL OF THE EUROPEAN CERAMIC SOCIETY. ISSN 0955-2219, 2018, vol. 38, no. 9, pp. 3154-3161., Registrované v: WOS

4. [1.1] ZVONAREV, S. V. - FROLOV, E. I. - SMIRNOV, N. O. - CHESNOKOV, K. Yu. Structure and Pulse Cathodoluminescence of Alumina Ceramic Doping with Magnesium. In PHYSICS, TECHNOLOGIES AND INNOVATION (PTI-2018). ISSN 0094-243X, 2018, vol. 2015, no., pp., Registrované v: WOS

ADCA103 DUSZA, Ján - ŠAJGALÍK, Pavol - REECE, Michael J. Analysis of Si₃N₄ + Beta-Si₃N₄ whisker ceramics. In Journal of Materials Science, 1991, vol. 26, p. 6782-6788. (1991 - Current Contents). ISSN 0022-2461.

Citácie:

1. [1.1] ZHANG, Wenliang - YI, Mingdong - XIAO, Guangchun - MA, Jun - WU, Guangyong - XU, Chonghai. Al₂O₃-coated h-BN composite powders and as-prepared Si₃N₄-based self-lubricating ceramic cutting tool material. In INTERNATIONAL JOURNAL OF REFRACTORY METALS & HARD MATERIALS. ISSN 0263-4368, 2018, vol. 71, no., pp. 1-7., Registrované v: WOS

ADCA104 DUSZA, Ján - ŠAJGALÍK, Pavol. Static fatigue resistance of Si₃N₄ + Si₃N₄ whisker ceramics at 1200 °C. In Journal of Materials Science Letters, 1994, vol. 13, p. 131-134. (1993: 0.490 - IF, karentované - CCC). (1994 - Current Contents). ISSN 0261-8028.

Citácie:

1. [1.1] XIE, Shaoxiong - XU, Jiageng - CHEN, Yu - TAN, Zhi - NIE, Rui - WANG, Qingyuan - ZHU, Jianguo. Flexural fracture mechanisms and fatigue behaviors of Bi₄Ti₃O₁₂-based high-temperature piezoceramics sintered at different temperatures. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 14, pp. 16758-16765., Registrované v: WOS

ADCA105 EGGER, David A. - RUIZ, Victor G. - SAID, Wissam A. - BUČKO, Tomáš - TKATCHENKO, Alexandre - ZOJER, Egbert. Understanding structure and bonding of multilayered metal-organic nanostructures. In Journal of Physical Chemistry C, 2013, vol. 117, no. 6, p. 3055-3061. (2012: 4.814 - IF, 2.514 - SJR, karentované - CCC). (2013 - Current Contents, WOS, SCOPUS). ISSN 1932-7447.

Citácie:

1. [1.1] VAN STRAATEN, Gerben - FRANKE, Markus - SOUBATCH, Serguei - STADTMUELLER, Benjamin - DUNCAN, David A. - LEE, Tien-Lin - TAUTZ, F. Stefan - KUMPF, Christian. Role of the Central Metal Atom in Substrate-Mediated Molecular Interactions in Phthalocyanine-Based Heteromolecular Monolayers. In JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, 2018, vol. 122, no. 15, pp. 8491-8504., Registrované v: WOS

2. [1.1] WANG, Qi - FRANCO-CANELLAS, Antoni - JI, Penghui - BUERKER, Christoph - WANG, Rong-Bin - BROCH, Katharina

- THAKUR, Pardeep Kumar - LEE, Tien-Lin - ZHANG, Haiming - GERLACH, Alexander - CHI, Lifeng - DUHM, Steffen - SCHREIBER, Frank. Bilayer Formation vs Molecular Exchange in Organic Heterostructures: Strong Impact of Subtle Changes in Molecular Structure. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 17, pp. 9480-9490., Registrované v: WOS

ADCA106 FAURE, Alexandre - VALIRON, Pierre - WERNLI, Michael - WIESENFELD, Laurent - RIST, Claire - NOGA, Jozef - TENNYSON, J. A full nine-dimensional potential-energy surface for hydrogen molecule-water collisions. In *Journal of Chemical Physics*, 2005, vol. 122, no. 22, p. 221102-1-221102-4. (2004: 3.105 - IF, karentované - CCC). (2005 - Current Contents, WOS, SCOPUS). ISSN 0021-9606.

Citácie:

1. [1.1] BORYSOW, Jacek - MORALDI, Massimo - NEUMANN, Martin. Calculation of the Raman Q branch of hydrogen in water and comparison with experiments. In *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*. ISSN 0953-4075, 2018, vol. 51, no. 23, pp., Registrované v: WOS

2. [1.1] SAHNOUN, E. - NKEM, C. - NAINDOUBA, A. - HAMMAMI, K. - JAIDANE, N. - OWONO, L. C. Owono. Quantum scattering of KCl with He/para-: potential energy surface and rate coefficients at low temperature. In *ASTROPHYSICS AND SPACE SCIENCE*. ISSN 0004-640X, 2018, vol. 363, no. 9, pp., Registrované v: WOS

ADCA107 FIDES, Martin - KOVALČÍKOVÁ, Alexandra - HVIZDOŠ, Pavol - BYSTRICKÝ, Roman - DŽUNDA, Róbert - BALKO, Ján - SEDLÁČEK, Jaroslav. Mechanical and tribological properties of electrically conductive SiC based cermets. In *International Journal of Refractory Metals and Hard Materials*, 2017, vol. 65, p. 76-82. (2016: 2.155 - IF, Q1 - JCR, 1.055 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0263-4368.

Citácie:

1. [1.1] CHO, Tae Young - MALIK, Rohit - KIM, Young Wook - KIM, Kwang Joo. Electrical and mechanical properties of pressureless sintered SiC-TiCN composites. In *Journal of the European Ceramic Society*. ISSN 09552219, 2018-08-01, 38, 9, pp. 3064-3072., Registrované v: WOS

ADCA108 FRAJKOROVÁ, Františka - HNATKO, Miroslav - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol. Electrically conductive silicon carbide with the addition of Ti-NbC. In *Journal of the European Ceramic Society*, 2012, vol. 32, no. 10, p. 2513-2518. (2011: 2.353 - IF, 1.343 - SJR, karentované - CCC). (2012 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] MALIK, Rohit - KIM, Hyun-Min - KIM, Young-Wook - KIM, Kwang Joo. Grain-growth-induced high electrical conductivity in SiC-BN composites. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 14, pp. 16394-16399., Registrované v: WOS

ADCA109 FRAJKOROVÁ, Františka - BODIŠOVÁ, Katarína - BOHÁČ, Martin - BARTONÍČKOVÁ, E. - SEDLÁČEK, Jaroslav. Preparation and characterisation of porous composite biomaterials based on silicon nitride and bioglass. In *Ceramics International*, 2015, vol. 41, no. 8, p. 9770-9778. (2014: 2.605 - IF, Q1 - JCR, 0.871 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] GUEDES-SILVA, Cecilia Chaves - DORION RODAS, Andrea Cecilia - SILVA, Antonio Carlos - RIBEIRO, Christiane - DE SOUZA CARVALHO, Flavio Machado - HIGA, Olga Zazuco - FERREIRA, Thiago dos Santos. Microstructure, Mechanical Properties and in vitro Biological Behavior of Silicon Nitride Ceramics. In *MATERIALS RESEARCH-IBERO-AMERICAN JOURNAL OF MATERIALS*. ISSN 1516-1439, 2018, vol. 21, no. 6, pp., Registrované v: WOS

ADCA110 FRIDRICHOVÁ, Jana - BAČÍK, Peter - RUSINOVÁ, Petra - ANTAL, Peter - ŠKODA, Radek - BIZOVSKÁ, Valéria - MIGLIERINI, Marcel. Optical and crystal-chemical changes in aquamarines and yellow beryls from Thanh Hoa province, Vietnam induced by heat treatment. In *Physics and chemistry of minerals*, 2015, vol. 42, p. 287-302. (2014: 1.538 - IF, Q2 - JCR, 0.756 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0342-1791.

Citácie:

1. [1.1] KADZIOŁKA-GAWEL, Mariola - DULSKI, Mateusz - KALINOWSKI, Lech - WOJTYNIAK, Marcin. The effect of gamma irradiation on the structural properties of olivine. In *JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY*. ISSN 0236-5731, 2018, vol. 317, no. 1, pp. 261-268., Registrované v: WOS

ADCA111 GALUSEK, Dušan - SEDLÁČEK, Jaroslav - CHOVANEK, Jozef - MICHÁLKOVÁ, Monika. The influence of MgO, Y₂O₃ and ZrO₂ additions on densification and grain growth of submicrometre alumina sintered by SPS and HIP. In *Ceramics International*, 2015, vol. 41, no. 8, p. 9692-9700. (2014: 2.605 - IF, Q1 - JCR, 0.871 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] WANG, Zhengjuan - ZHOU, Guohong - JIANG, Danyu - WANG, Shiwei. Recent development of A(2)B(2)O(7) system transparent ceramics. In *JOURNAL OF ADVANCED CERAMICS*. ISSN 2226-4108, 2018, vol. 7, no. 4, pp. 289-306., Registrované v: WOS

2. [1.1] YU, Hui - XU, Zhihao - WEI, Ziyi - CHEN, Yongjun - LI, Jianbao - LUO, Lijie. Effect of talc and titania on the microstructure and mechanical properties of alumina ceramics. In *INTERNATIONAL JOURNAL OF APPLIED CERAMIC TECHNOLOGY*. ISSN 1546-542X, 2018, vol. 15, no. 3, pp. 633-642., Registrované v: WOS

ADCA112 GALUSEK, Dušan - GALUSKOVÁ, Dagmar. Alumina matrix composites with non-oxide nanoparticle addition and enhanced functionalities. In *NANOMATERIALS-BASEL*, 2015, vol. 5, no.

1, p. 115-143. (2014: 2.076 - IF, Q2 - JCR, karentované - CCC). (2015 - Current Contents). ISSN 2079-4991.

Citácie:

1. [1.1] HALDER, Rupa - SARKAR, Soumya - BANDYOPADHYAY, Siddhartha - CHAKRABORTI, Pravash C. Sintering and tribomechanical properties of gel-combustion-derived nano-alumina and its composites with carbon nanotubes. In *JOURNAL OF MATERIALS SCIENCE*. ISSN 0022-2461, 2018, vol. 53, no. 12, pp. 8989-9001., Registrované v: WOS
2. [1.1] SAHEB, N. - MOHAMMAD, K. Hard and tough Al₂O₃-SiC-CNT hybrid ceramic nanocomposite produced by molecular level mixing and spark plasma sintering. In *JOURNAL OF THE AUSTRALIAN CERAMIC SOCIETY*. ISSN 2510-1560, 2018, vol. 54, no. 3, pp. 401-410., Registrované v: WOS
3. [1.1] SANGEETHA, M. - PRAKASH, S. - JAYAPRAKASH - RAGHAVENDRA, Kotra - MITHUN, M. Mechanical Survey and Morphological Review of LM22 composite Coated with Multi Wall Carbon Nano Tubes. In *MATERIALS TODAY-PROCEEDINGS*. ISSN 2214-7853, 2018, vol. 5, no. 11, pp. 24924-24928., Registrované v: WOS

ADCA113 GALUSEK, Dušan - TWIGG, P.C. - RILEY, F.L. Wet erosion of liquid phase sintered alumina. In *Wear : an international journal on the science and technology of friction, lubrication and wear*, 1999, vol. 233-235, p. 588-595. ISSN 0043-1648.

Citácie:

1. [1.1] KLEGUES MONTEDO, Oscar Rubem - MILAK, Pamela Cabreira - FALLER, Cristian Arnaldo - PETERSON, Michael - DE NONI JUNIOR, Agenor. Effect of LZSA Glass-Ceramic Addition on Pressureless Sintered Alumina. Part II: Mechanical Behavior. In *MATERIALS RESEARCH-IBERO-AMERICAN JOURNAL OF MATERIALS*. ISSN 1516-1439, 2018, vol. 21, no. 1, pp., Registrované v: WOS

ADCA114 GALUSEK, Dušan - RILEY, F.L. - RIEDEL, Ralf. Nanoindentation of a polymer-derived amorphous silicon carbonitride ceramic. In *Journal of the American Ceramic Society*, 2001, vol. 84, no. 5, p. 1164-1166. (2000: 2.017 - IF, karentované - CCC). (2001 - Current Contents). ISSN 0002-7820.

Citácie:

1. [1.1] FONBLANC, Diane - LOPEZ-FERBER, David - WYNN, Melanie - LALE, Abhijeet - SOLEILHAVOUP, Anne - LERICHE, Anne - IWAMOTO, Yuji - ROSSIGNOL, Fabrice - GERVAIS, Christel - BERNARD, Samuel. Crosslinking chemistry of poly(vinylmethyl-co-methyl)silazanes toward low-temperature formable preceramic polymers as precursors of functional aluminium-modified Si-C-N ceramics. In *DALTON TRANSACTIONS*. ISSN 1477-9226, 2018, vol. 47, no. 41, pp. 14580-14593., Registrované v: WOS
2. [1.1] GOWAYED, Y. - PIERCE, J. - BUCHANAN, D. - ZAWADA, L. - JOHN, R. - DAVIDSON, K. Effect of microstructural features and properties of constituents on the thermo-elastic properties of ceramic matrix composites. In *COMPOSITES PART B-ENGINEERING*. ISSN 1359-8368, 2018, vol. 135, no., pp. 155-165., Registrované v: WOS
3. [1.1] JIA, Dechang - LIANG, Bin - YANG, Zhihua - ZHOU, Yu. Metastable Si-B-C-N ceramics and their matrix composites developed by inorganic route based on mechanical alloying: Fabrication, microstructures, properties and their relevant basic scientific issues. In *PROGRESS IN MATERIALS SCIENCE*. ISSN 0079-6425, 2018, vol. 98, no., pp. 1-67., Registrované v: WOS
4. [1.1] MA, Benyuan - ZHANG, Wei - WANG, Yuezong - SONG, Haizhi - XIE, Xiumin - ZHANG, Zhibin - YAO, Chao - LUO, Hui - NIU, Ruihua. Fabrication and nanoindentation characterization of MgAlON transparent ceramics. In *OPTICAL MATERIALS*. ISSN 0925-3467, 2018, vol. 84, no., pp. 714-721., Registrované v: WOS

ADCA115 GALUSEK, Dušan - RESCHKE, S. - RIEDEL, Ralf - DRESSLER, W. - MAJLING, J. - ŠAJGALÍK, Pavol - LENČEŠ, Zoltán. In-situ carbon content adjustment in polysilazane derived amorphous SiCN bulk ceramics. In *Journal of the European Ceramic Society*, 1999, vol. 19, no. 10, p. 1911-1921.

Citácie:

1. [1.1] WANG, Qi - YANG, Mei - XIAO, Jiusan - JIAO, Shuqiang - ZHU, Hongmin. Synthesis, characterization and sintering of Si-C-N nano-powders via sodium reduction in liquid ammonia. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 4, pp. 1219-1226., Registrované v: WOS

ADCA116 GALUSEK, Dušan - GHILLÁNYOVÁ, Katarína - SEDLÁČEK, Jaroslav - KOZÁNKOVÁ, Jana - ŠAJGALÍK, Pavol. The influence of additives on microstructure of sub-micron alumina ceramics prepared by two-stage sintering. In *Journal of the European Ceramic Society*, 2012, vol. 32, no. 9, p. 1965-1970. (2011: 2.353 - IF, 1.343 - SJR, karentované - CCC). (2012 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] DMITRIEVSKII, A. A. - TYURIN, A. I. - ZHIGACHEV, A. O. - GUSEVA, D. G. - OVCHINNIKOV, P. N. The Influence of Corundum Content and Sintering Temperature on the Mechanical Properties of CaO-ZrO₂-Al₂O₃ Ceramic Composites. In *TECHNICAL PHYSICS LETTERS*. ISSN 1063-7850, 2018, vol. 44, no. 2, pp. 141-144., Registrované v: WOS

ADCA117 GALUSKOVÁ, Dagmar - KAŠIAROVÁ, Monika - HNATKO, Miroslav - GALUSEK, Dušan - DUSZA, Ján - ŠAJGALÍK, Pavol. Hydrothermal corrosion and flexural strength of Si₃N₄-based ceramics. In *Corrosion Science*, 2014, vol. 85, p. 94-100. (2013: 3.686 - IF, 1.592 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 0010-938X.

Citácie:

1. [1.1] ARAI, Masatsugu. Degradation of bending strength occurred by corrosion of sintered silicon nitride in aqueous acidic solutions. In *MECHANICAL ENGINEERING JOURNAL*. ISSN 2187-9745, 2018, vol. 5, no. 2, pp., Registrované v: WOS
2. [1.1] WU, Jianfeng - HU, Cheng - PING, Chen - XU, Xiaohong - XIANG, Weiheng. Preparation and corrosion resistance of cordierite-spodumene composite ceramics using zircon as a modifying agent. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 16, pp. 19590-19596., Registrované v: WOS
3. [1.1] ZHANG, Wenliang - YI, Mingdong - XIAO, Guangchun - MA, Jun - WU, Guangyong - XU, Chonghai. Al₂O₃-coated h-BN composite powders and as-prepared Si₃N₄-based self-lubricating ceramic cutting tool material. In *INTERNATIONAL JOURNAL OF REFRACTORY METALS & HARD MATERIALS*. ISSN 0263-4368, 2018, vol. 71, no., pp. 1-7., Registrované v: WOS

- ADCA118 GAMBÁ, Martina - FLORES, Federico M. - MADEJOVÁ, Jana - TORRES SÁNCHEZ, Rosa M. Comparison of imazalil removal onto montmorillonite and nanomontmorillonite and adsorption surface sites involved: an approach for agricultural wastewater treatment. In *Industrial & Engineering Chemistry Research*, 2015, vol. 54, no. 5, p. 1529-1538. (2014: 2.587 - IF, Q1 - JCR, 1.012 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0888-5885.

Citácie:

1. [1.1] ZHANG, Liang - LYU, Tao - VARGAS, Carlos Andres Ramirez - ARIAS, Carlos A. - CARVALHO, Pedro N. - BRIX, Hans. New insights into the effects of support matrix on the removal of organic micro-pollutants and the microbial community in constructed wetlands. In *ENVIRONMENTAL POLLUTION*. ISSN 0269-7491, 2018, vol. 240, no., pp. 699-708., Registrované v: WOS

- ADCA119 GATES, W.P. - KOMADEL, Peter - MADEJOVÁ, Jana - BUJDÁK, Juraj - STUCKI, Joseph W. - KIRKPATRICK, R.J. Electronic and structural properties of reduced-charge montmorillonites. In *Applied Clay Science*, 2000, vol. 16, no. 5-6, p. 257-271.

Citácie:

1. [1.1] BODART, Philippe R. - DELMOTTE, L. - RIGOLET, S. - BRENDLE, J. - GOUGEON, Regis D. Li-7{F-19} TEDOR NMR to observe the lithium migration in heated montmorillonite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 157, no., pp. 204-211., Registrované v: WOS

2. [1.1] GIL REBAZA, A. V. - MONTES, M. L. - TAYLOR, M. A. - ERRICO, L. A. - ALONSO, R. E. Experimental and theoretical study of Co sorption in clay montmorillonites. In *MATERIALS RESEARCH EXPRESS*. ISSN 2053-1591, 2018, vol. 5, no. 3, pp., Registrované v: WOS

3. [1.1] MAHMOODI, Syed Muhammad Ibad - PADMANABHAN, Eswaran. Hydrocarbon Bond Variation in Some Shales from Batu Gajah, Malaysia. In *ICIPEG 2016: PROCEEDINGS OF THE INTERNATIONAL CONFERENCE ON INTEGRATED PETROLEUM ENGINEERING AND GEOSCIENCES*, 2017, vol., no., pp. 363-371., Registrované v: WOS

4. [1.1] SHEN, Wei - LI, Lin - ZHOU, Huijun - ZHOU, Qing - CHEN, Meng - ZHU, Jianxi. Effects of charge density on the hydration of siloxane surface of montmorillonite: A molecular dynamics simulation study. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 159, no., pp. 10-15., Registrované v: WOS

- ADCA120 GEDEON, Ondrej - LIŠKA, Marek - MACHÁČEK, Jan. Volume fluctuations in potassium silicate glass studied by molecular dynamics. In *Journal of Non-Crystalline Solids*, 2011, vol. 357, no. 6-7, p. 1574-1581. (2010: 1.492 - IF, karentované - CCC). (2011 - Current Contents, SCOPUS). ISSN 0022-3093.

Citácie:

1. [1.1] SUN, Yicheng - ZHOU, Huiqun - YIN, Kun - ZHAO, Mengqi - XU, Shijin - LU, Xiancai. Transport Properties of Fe₂SiO₄ Melt at High Pressure From Classical Molecular Dynamics: Implications for the Lifetime of the Magma Ocean. In *JOURNAL OF GEOPHYSICAL RESEARCH-SOLID EARTH*. ISSN 2169-9313, 2018, vol. 123, no. 5, pp. 3667-3679., Registrované v: WOS

- ADCA121 GEDEON, Ondrej - LIŠKA, Marek - MACHÁČEK, Jan. Connectivity of Q-species in binary sodium-silicate glasses. In *Journal of Non-Crystalline Solids*, 2008, vol. 354, no. 12-13, p. 1133-1136. (2007: 1.319 - IF, karentované - CCC). (2008 - Current Contents, SCOPUS). ISSN 0022-3093.

Citácie:

1. [1.1] SHIN, S. H. - JEONG, Y. C. - CHO, J. W. - KIM, S. H. Highlighting a rheological behavior of glass melt at high temperature. In *JOURNAL OF NON-CRYSTALLINE SOLIDS*. ISSN 0022-3093, 2018, vol. 499, no., pp. 41-48., Registrované v: WOS

- ADCA122 GÖLTL, Florian - GRÜNEIS, Andreas - BUČKO, Tomáš - HAFNER, Jürgen. Van der Waals interactions between hydrocarbon molecules and zeolites: Periodic calculations at different levels of theory, from density functional theory to the random phase approximation and Møller-Plesset perturbation theory. In *Journal of Chemical Physics*, 2012, vol. 137, no. 11, p. 114111-1-114111-17. (2011: 3.333 - IF, 1.805 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] ALESSIO, Maristella - BISCHOFF, Florian A. - SAUER, Joachim. Chemically accurate adsorption energies for methane and ethane monolayers on the MgO(001) surface. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 15, pp. 9760-9769., Registrované v: WOS

2. [1.1] FANG, Hanjun - AWATI, Rohan - BOULFELFEL, Salah E. - RAVIKOVITCH, Peter I. - SHOLL, David S. First-Principles-Derived Force Fields for CH₄ Adsorption and Diffusion in Siliceous Zeolites. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 24, pp. 12880-12891., Registrované v: WOS

3. [1.1] GATTA, G. D. - LOTTI, P. - TABACCHI, G. The effect of pressure on open-framework silicates: elastic behaviour and crystal-fluid interaction. In *PHYSICS AND CHEMISTRY OF MINERALS*. ISSN 0342-1791, 2018, vol. 45, no. 2, pp. 115-138., Registrované v: WOS

4. [1.1] GRAJCIAR, Lukas - HEARD, Christopher J. - BONDARENKO, Anton A. - POLYNSKI, Mikhail V. - MEEPRASERT, Jittima - PIDKO, Evgeny A. - NACHTIGALL, Petr. Towards operando computational modeling in heterogeneous catalysis. In *CHEMICAL SOCIETY REVIEWS*. ISSN 0306-0012, 2018, vol. 47, no. 22, pp. 8307-8348., Registrované v: WOS

5. [1.1] HESSOU, E. P. - KANHOUNNON, W. G. - ROCCA, D. - MONNIER, H. - VALLIERES, C. - LEBEGUE, S. - BADAWI, M. Adsorption of NO, NO₂, CO, H₂O and CO₂ over isolated monovalent cations in faujasite zeolite: a periodic DFT investigation. In *THEORETICAL CHEMISTRY ACCOUNTS*. ISSN 1432-881X, 2018, vol. 137, no. 12, pp., Registrované v: WOS

6. [1.1] MAESTRI, Matteo - IGLESIA, Enrique. First-principles theoretical assessment of catalysis by confinement: NO-O₂ reactions within voids of molecular dimensions in siliceous crystalline frameworks. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 23, pp. 15725-15735., Registrované v: WOS

7. [1.1] PICCINI, GiovanniMaria - ALESSIO, Maristella - SAUER, Joachim. Ab initio study of methanol and ethanol adsorption on Brønsted sites in zeolite H-MFI. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 30, pp. 19964-19970., Registrované v: WOS

8. [1.1] PLESSOW, Philipp N. - STUDDT, Felix. *Theoretical Insights into the Effect of the Framework on the Initiation Mechanism of the MTO Process*. In CATALYSIS LETTERS. ISSN 1011-372X, 2018, vol. 148, no. 4, pp. 1246-1253., Registrované v: WOS
9. [1.1] SCHAEFER, Tobias - RAMBERGER, Benjamin - KRESSE, Georg. *Laplace transformed MP2 for three dimensional periodic materials using stochastic orbitals in the plane wave basis and correlated sampling*. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 6, pp., Registrované v: WOS

ADCA123 GOULD, Tim - BUČKO, Tomáš. C6 coefficients and dipole polarizabilities for all atoms and many ions in rows 1-6 of the periodic table. In Journal of Chemical Theory and Computation, 2016, vol. 12, p. 3603-3613. (2015: 5.301 - IF, Q1 - JCR, 2.702 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 1549-9618.

Citácie:

1. [1.1] ALDERMAN, O. L. G. - BENMORE, C. J. - NEUEFEIND, J. - COILLET, E. - MERMET, A. - MARTINEZ, V. - TAMALONIS, A. - WEBER, R. *Amorphous tantalum and its relationship with the molten state*. In PHYSICAL REVIEW MATERIALS. ISSN 2475-9953, 2018, vol. 2, no. 4, pp., Registrované v: WOS
2. [1.1] BERWANGER, Julian - HUBER, Ferdinand - STILP, Fabian - GIESSIBL, Franz J. *Lateral manipulation of single iron adatoms by means of combined atomic force and scanning tunneling microscopy using CO-terminated tips*. In PHYSICAL REVIEW B. ISSN 2469-9950, 2018, vol. 98, no. 19, pp., Registrované v: WOS
3. [1.1] BUENO-PEREZ, Rocio - BALESTRA, Salvador R. G. - CAMBLOR, Miguel A. - MIN, Jung Gi - HONG, Suk Bong - MERKLING, Patrick J. - CALERO, Sofia. *Influence of Flexibility on the Separation of Chiral Isomers in STW-Type Zeolite*. In CHEMISTRY-A EUROPEAN JOURNAL. ISSN 0947-6539, 2018, vol. 24, no. 16, pp. 4121-4132., Registrované v: WOS
4. [1.1] FEDOROV, Dmitry - SADHUKHAN, Mainak - STOEHR, Martin - TKATCHENKO, Alexandre. *Quantum-Mechanical Relation between Atomic Dipole Polarizability and the van der Waals Radius*. In PHYSICAL REVIEW LETTERS. ISSN 0031-9007, 2018, vol. 121, no. 18, pp., Registrované v: WOS
5. [1.1] HEIDAR-ZADEH, Farnaz - AYERS, Paul W. - VERSTRAELEN, Toon - VINOGRADOV, Ivan - VOHRINGER-MARTINEZ, Esteban - BULTINCK, Patrick. *Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes*. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 17, pp. 4219-4245., Registrované v: WOS
6. [1.1] JERABEK, Paul - SCHWERTDFEGER, Peter - NAGLE, Jeffrey K. *Static dipole polarizability of palladium from relativistic coupled-cluster theory*. In PHYSICAL REVIEW A. ISSN 2469-9926, 2018, vol. 98, no. 1, pp., Registrované v: WOS
7. [1.1] RIQUELME, Maximilian - LARA, Alejandro - MOBLEY, David L. - VERSTRAELEN, Toon - MATAMALA, Adelio R. - VOHRINGER-MARTINEZ, Esteban. *Hydration Free Energies in the FreeSolv Database Calculated with Polarized Iterative Hirshfeld Charges*. In JOURNAL OF CHEMICAL INFORMATION AND MODELING. ISSN 1549-9596, 2018, vol. 58, no. 9, pp. 1779-1797., Registrované v: WOS

ADCA124 GOULD, Tim - LEBÈGUE, Sébastien - ÁNGYÁN, János G. - BUČKO, Tomáš. A fractionally ionic approach to polarizability and van der Waals many-body dispersion calculations. In Journal of Chemical Theory and Computation, 2016, vol. 12, no. 12, p. 5920-5930. (2015: 5.301 - IF, Q1 - JCR, 2.702 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 1549-9618.

Citácie:

1. [1.1] BEDOYA-MARTINEZ, Natalia - GIUNCHI, Andrea - SALZILLO, Tommaso - VENUTI, Elisabetta - DELLA VALLE, Raffaele Guido - ZOJER, Egbert. *Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions*. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 8, pp. 4380-4390., Registrované v: WOS
2. [1.1] HEIDAR-ZADEH, Farnaz - AYERS, Paul W. - VERSTRAELEN, Toon - VINOGRADOV, Ivan - VOHRINGER-MARTINEZ, Esteban - BULTINCK, Patrick. *Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes*. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 17, pp. 4219-4245., Registrované v: WOS
3. [1.1] HESSELMANN, Andreas - MEITEI, Oinam Romesh. *Intermolecular dispersion energies from coupled exact-exchange Kohn-Sham excitation energies and vectors*. In COMPUTATIONAL AND THEORETICAL CHEMISTRY. ISSN 2210-271X, 2018, vol. 1129, no., pp. 57-69., Registrované v: WOS
4. [1.1] HESSELMANN, Andreas. *Geometry optimisations with a nonlocal density-functional theory method based on a double Hirshfeld partitioning*. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 4, pp., Registrované v: WOS
5. [1.1] LOBODA, Oleksandr A. - DOLGONOS, Goryoriy A. - BOESE, A. Daniel. *Towards hybrid density functional calculations of molecular crystals via fragment-based methods*. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 12, pp., Registrované v: WOS
6. [1.1] SROUR, Juliana - BADAWI, Michael - HASSAN, Fouad El Haj - POSTNIKOV, Andrei. *Comparative study of structural and electronic properties of GaSe and InSe polytypes*. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 5, pp., Registrované v: WOS
7. [1.1] TAO, Jianmin - PERDEW, John P. - TANG, Hong - SHAHI, Chandra. *Origin of the size-dependence of the equilibrium van der Waals binding between nanostructures*. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 7, pp., Registrované v: WOS
8. [1.1] TERENTJEV, Aleksandr - CONSTANTIN, Lucian A. - PITARKE, J. M. *Dispersion-corrected PBEsol exchange-correlation functional*. In PHYSICAL REVIEW B. ISSN 2469-9950, 2018, vol. 98, no. 21, pp., Registrované v: WOS
9. [1.1] WIEME, J. - LEJAEGHERE, K. - KRESSE, G. - VAN SPEYBROECK, V. *Tuning the balance between dispersion and entropy to design temperature-responsive flexible metal-organic frameworks*. In NATURE COMMUNICATIONS. ISSN 2041-1723, 2018, vol. 9, no., pp., Registrované v: WOS

ADCA125 GREGUŠOVÁ, Adriana - ČERNUŠÁK, Ivan - MALKINA, Olga - NOGA, Jozef. On the structure and stability of cyclic cyanoborane isomers. In Physical Chemistry Chemical Physics, 2003, vol. 5, no. 19, p. 4084-4089. ISSN 1463-9076.

Citácie:

1. [1.1] MANNA, Shovan - RAY, Suvonil Sinha - GHOSH, Pradipta - CHATTOPADHYAY, Sudip. On the conversion XCN <-> XNC via an efficient and economic perturbative wave function approach. In *MOLECULAR PHYSICS*. ISSN 0026-8976, 2018, vol. 116, no. 17, pp. 2147-2161., Registrované v: WOS

ADCA126 GROSSMANN, Gisbert - OHMS, Gisela - KRÜGER, Kerstin - KARAGHIOSOFF, Konstantin - ECKSTEIN, Klaus - HAHN, Josef - HOPP, Andreas - MALKINA, Ol'ga - HROBÁRIK, Peter. Diselenadiphosphetane diselenides and triselenadiphospholane diselenides - synthesis and characterization by ³¹P and ⁷⁷Se solid-state NMR spectroscopy. In *Zeitschrift für Anorganische und Allgemeine Chemie*, 2001, vol. 627, no. 6, p. 1269-1278. ISSN 0044-2313.

Citácie:

1. [1.1] ARISAWA, Mieko - SAWAHATA, Kyosuke - YAMADA, Tomoki - SARKAR, Debayan - YAMAGUCHI, Masahiko. Rhodium-Catalyzed Insertion Reaction of PhP Group of Pentaphenylcyclopentaphosphine with Acyclic and Cyclic Disulfides. In *ORGANIC LETTERS*. ISSN 1523-7060, 2018, vol. 20, no. 4, pp. 938-941., Registrované v: WOS

ADCA127 HAASE, Pi A. B. - REPISKÝ, Michal - KOMOROVSKÝ, Stanislav - BENDIX, Jesper - SAUER, Stephan P. A. Relativistic DFT calculations of hyperfine coupling constants in 5d hexafluorido complexes: [ReF₆]²⁻ and [IrF₆]²⁻. In *Chemistry - A European Journal*, 2018, vol. 24, no. 20, p. 5124-5133. (2017: 5.160 - IF, Q1 - JCR, 2.265 - SJR, Q1 - SJR, karentované - CCC). (2018 - Current Contents). ISSN 0947-6539.

Citácie:

1. [1.1] KRIVDIN, Leonid B. Theoretical calculations of carbon-hydrogen spin-spin coupling constants. In *PROGRESS IN NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY*. ISSN 0079-6565, 2018, vol. 108, no., pp. 17-73., Registrované v: WOS

ADCA128 HALADEJOVÁ, Katarína - PRNOVÁ, Anna - KLEMENT, Róbert - TUAN, Wei-Hsing - SHIH, S. J. - GALUSEK, Dušan. Aluminate glass based phosphors for LED applications. In *Journal of the European Ceramic Society*, 2016, vol. 36, no. 12, p. 2969-2973. (2015: 2.933 - IF, Q1 - JCR, 1.150 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0955-2219.

Citácie:

1. [1.1] ZHANG, Yunli - HU, Song - WANG, Zhengjuan - ZHOU, Guohong - WANG, Shiwei. Pore-existing Lu₃Al₅O₁₂:Ce ceramic phosphor: An efficient green color converter for laser light source. In *JOURNAL OF LUMINESCENCE*. ISSN 0022-2313, 2018, vol. 197, no., pp. 331-334., Registrované v: WOS

ADCA129 HALIAKOVÁ, Anna - PRNOVÁ, Anna - KLEMENT, Róbert - GALUSEK, Dušan - TUAN, Wei-Hsing. Flame-spraying synthesis of aluminate glasses in the Al₂O₃-La₂O₃ system. In *Ceramics International*, 2012, vol. 38, no. 7, p. 5543-5549. (2011: 1.751 - IF, 0.922 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] LI, Xiaoyu - MA, Xiaoguang - LI, Jiangtao - HE, Gang - LI, Jianqiang. Synthesis of amorphous La₄Ti₉O₂₄ microspheres with high-refractive index via containerless flame-spraying method. In *MATERIALS RESEARCH BULLETIN*. ISSN 0025-5408, 2018, vol. 97, no., pp. 567-571., Registrované v: WOS

ADCA130 HANZEL, Ondrej - SEDLÁK, Richard - SEDLÁČEK, Jaroslav - BIZOVSKÁ, Valéria - BYSTRICKÝ, Roman - GIRMAN, Vladimír - KOVALČÍKOVÁ, Alexandra - DUSZA, Ján - ŠAJGALÍK, Pavol. Anisotropy of functional properties of SiC composites with GNPs, GO and in-situ formed graphene. In *Journal of the European Ceramic Society*, 2017, vol. 37, p. 3731-3739. (2016: 3.454 - IF, Q1 - JCR, 1.142 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0955-2219.

Citácie:

1. [1.1] HAN, Meizhao - LI, Jing - MUHAMMAD, Yaseen - HOU, Dianhao - ZHANG, Fenglei - YIN, Yuhua - DUAN, Shaochan. Effect of polystyrene grafted graphene nanoplatelets on the physical and chemical properties of asphalt binder. In *CONSTRUCTION AND BUILDING MATERIALS*. ISSN 0950-0618, 2018, vol. 174, no., pp. 108-119., Registrované v: WOS

2. [1.1] HUANG YI-HUA - JIANG DONG-LIANG - CHEN ZHONG-MING - LIU XUE-JIAN - ZHANG XIAN-FENG - LIAO ZHEN-KUI - HUANG ZHENG-REN. Fabrication and Property of rGO/SiC Composite. In *JOURNAL OF INORGANIC MATERIALS*. ISSN 1000-324X, 2018, vol. 33, no. 11, pp. 1147-1153., Registrované v: WOS

3. [1.1] HUANG YIHUA - JIANG DONGLIANG - ZHANG XIANFEN - LIAO ZHENKUI - HUANG ZHENGREN. Enhancing toughness and strength of SiC ceramics with reduced graphene oxide by HP sintering. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 13, pp. 4329-4337., Registrované v: WOS

4. [1.1] POYATO, R. - OSUNA, J. - MORALES-RODRIGUEZ, A. - GALLARDO-LOPEZ, A. Electrical conduction mechanisms in graphene nanoplatelet/yttria tetragonal zirconia composites. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 12, pp. 14610-14616., Registrované v: WOS

5. [1.1] SUN, Mengyong - BAI, Yuhang - LI, Mingxing - FAN, Shangwu - CHENG, Laifei. Improved toughness and electromagnetic shielding-effectiveness for graphite-doped SiC ceramics with a net-like structure. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 16, pp. 5271-5281., Registrované v: WOS

6. [1.1] WIECLAW-MIDOR, A. - WIECINSKA, P. - SZAFRAN, M. Surface Modification of Alumina Powder to Prevent Exfoliation of Samples Fabricated by Gelcasting. In *JOURNAL OF CERAMIC SCIENCE AND TECHNOLOGY*. ISSN 2190-9385, 2018, vol. 9, no. 3, pp. 225-233., Registrované v: WOS

ADCA131 HANZEL, Ondrej - LOFAJ, František - SEDLÁČEK, Jaroslav - KABÁTOVÁ, Margita - KAŠIAROVÁ, Monika - ŠAJGALÍK, Pavol. Mechanical and tribological properties of alumina-MWCNTs composites sintered by rapid hot-pressing. In *Journal of the European Ceramic Society*, 2017, vol. 37, no. 15, p. 4821-4831. (2016: 3.454 - IF, Q1 - JCR, 1.142 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0955-2219.

Citácie:

1. [1.1] EL SHALAKANY, Abou Bakr - KAMEL, Bahaa M. - KHATTAB, A. - OSMAN, T. A. - AZZAM, B. - ZAKI, M. Improved mechanical and tribological properties of A356 reinforced by MWCNTs. In FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES. ISSN 1536-383X, 2018, vol. 26, no. 4, pp. 185-194., Registrované v: WOS
- ADCA132 HANZEL, Ondrej - SEDLÁČEK, Jaroslav - HADZIMOVÁ, Eva - ŠAJGALÍK, Pavol. Thermal properties of alumina-MWCNTs composites. In Journal of the European Ceramic Society, 2015, vol. 35, no. 5, p. 1559-1567. (2014: 2.947 - IF, Q1 - JCR, 1.187 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0955-2219.
- Citácie:
1. [1.1] AHMAD, Iftikhar - SUBHANI, Tayyab - WANG, Nannan - ZHU, Yanqiu. Thermophysical Properties of High-Frequency Induction Heat Sintered Graphene Nanoplatelets/Alumina Ceramic Functional Nanocomposites. In JOURNAL OF MATERIALS ENGINEERING AND PERFORMANCE. ISSN 1059-9495, 2018, vol. 27, no. 6, pp. 2949-2959., Registrované v: WOS
 2. [1.1] SINGH, Meinam Annebushan - SARNIA, Deba Kumar. Parametric and subsurface analysis of MWCNT alumina composites in WEDM process. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 2, pp. 2186-2197., Registrované v: WOS
- ADCA133 HANZEL, Ondrej - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. New approach for distribution of carbon nanotubes in alumina matrix. In Journal of the European Ceramic Society, 2014, vol. 34, no. 7, p. 1845-1851. (2013: 2.307 - IF, 1.122 - SJR, karentované - CCC). (2014 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.
- Citácie:
1. [1.1] HALDER, Rupa - SARKAR, Soumya - BANDYOPADHYAY, Siddhartha - CHAKRABORTI, Pravash C. Sintering and tribomechanical properties of gel-combustion-derived nano-alumina and its composites with carbon nanotubes. In JOURNAL OF MATERIALS SCIENCE. ISSN 0022-2461, 2018, vol. 53, no. 12, pp. 8989-9001., Registrované v: WOS
 2. [1.1] KOCJAN, Andraz - SCHMIDT, Rainer - LAZAR, Ana - PRADO-GONJAL, Jesus - KOVAC, Janez - LOGAR, Manca - MOMPEAN, Francisco J. - GARCIA-HERNANDEZ, Mar - RUIZ-HITZKY, Eduardo - WICKLEIN, Bernd. In situ generation of 3D graphene-like networks from cellulose nanofibres in sintered ceramics. In NANOSCALE. ISSN 2040-3364, 2018, vol. 10, no. 22, pp. 10488-10497., Registrované v: WOS
 3. [1.1] LEONOV, A. A. - KHASANOV, A. O. - DANCHENKO, V. A. - KHASANOV, O. L. Spark plasma sintering of ceramic matrix composite based on alumina, reinforced by carbon nanotubes. In INTERNATIONAL CONFERENCE MODERN TECHNOLOGIES AND MATERIALS OF NEW GENERATIONS. ISSN 1757-8981, 2018, vol. 286, no., pp., Registrované v: WOS
 4. [1.1] SINGH, Meinam Annebushan - SARNIA, Deba Kumar. Parametric and subsurface analysis of MWCNT alumina composites in WEDM process. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 2, pp. 2186-2197., Registrované v: WOS
- ADCA134 HELGAKER, Trygve - KLOPPER, Wim - KOCH, Henrik - NOGA, Jozef. Basis-set convergence of correlated calculations on water. In Journal of Chemical Physics, 1997, vol. 106, no. 23, p. 9639-9646. (1996: 3.516 - IF, karentované - CCC). (1997 - Current Contents, WOS, SCOPUS, WOS, SCOPUS). ISSN 0021-9606.
- Citácie:
1. [1.1] ABBOTT, Adam S. - GLICK, Zach L. - SCHAEFER, Henry F. Reinterpretation of the electronic absorption spectrum of the methylene amidogen radical (H₂CN). In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 9, pp., Registrované v: WOS
 2. [1.1] ABBOTT, Adam S. - SCHAEFER, Henry F. The Structure and Cl-O Dissociation Energy of the ClOO Radical: Finally, the Right Answers for the Right Reason. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 9, pp. 2604-2610., Registrované v: WOS
 3. [1.1] ABE, M. - PRASANNA, V. S. - DAS, B. P. Application of the finite-field coupled-cluster method to calculate molecular properties relevant to electron electric-dipole-moment searches. In PHYSICAL REVIEW A. ISSN 2469-9926, 2018, vol. 97, no. 3, pp., Registrované v: WOS
 4. [1.1] ALESSANDRINI, Silvia - GAUSS, Juergen - PUZZARINI, Cristina. Accuracy of Rotational Parameters Predicted by High-Level Quantum-Chemical Calculations: Case Study of Sulfur-Containing Molecules of Astrochemical Interest. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 10, pp. 5360-5371., Registrované v: WOS
 5. [1.1] ALESSIO, Maristella - BISCHOFF, Florian A. - SAUER, Joachim. Chemically accurate adsorption energies for methane and ethane monolayers on the MgO(001) surface. In PHYSICAL CHEMISTRY CHEMICAL PHYSICS. ISSN 1463-9076, 2018, vol. 20, no. 15, pp. 9760-9769., Registrované v: WOS
 6. [1.1] BABBUS, Ryan - WIEBE, Nathan - MCCLEAN, Jarrod - MCCLAIN, James - NEVEN, Hartmut - CHAN, Garnet Kin-Lic. Low-Depth Quantum Simulation of Materials. In PHYSICAL REVIEW X. ISSN 2160-3308, 2018, vol. 8, no. 1, pp., Registrované v: WOS
 7. [1.1] BALANCA, Christian - DAYOU, Fabrice - FAURE, Alexandre - WIESENFELD, Laurent - FEAUTRIER, Nicole. Rotationally inelastic collisions of SiO with H-2. In MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY. ISSN 0035-8711, 2018, vol. 479, no. 2, pp. 2692-2701., Registrované v: WOS
 8. [1.1] BARCLAY, A. J. - CHARMET, A. Pietropoli - MICHAELIAN, K. H. - MOAZZEN-AHMADI, N. Characterization of OCS-HCCCCH and N2O-HCCCCH Dimers: Theory and Experiment. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 24, pp. 5383-5390., Registrované v: WOS
 9. [1.1] BARTLETT, Marcus A. - LIANG, Tao - PU, Liang - SCHAEFER, Henry F. - ALLEN, Wesley D. The multichannel n-propyl + O-2 reaction surface: Definitive theory on a model hydrocarbon oxidation mechanism. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 9, pp., Registrované v: WOS
 10. [1.1] BASSETT, Matthew K. - FORTENBERRY, Ryan C. Magnesium replacement in formaldehyde: Theoretical rovibrational analysis of (X)over-tilde B-3(1) MgCH2. In JOURNAL OF MOLECULAR SPECTROSCOPY. ISSN 0022-2852, 2018, vol. 344, no., pp. 61-64., Registrované v: WOS
 11. [1.1] BAUSCHLICHER, Charles W. The convergence of the coupled cluster approach for MgO. In CHEMICAL PHYSICS LETTERS. ISSN 0009-2614, 2018, vol. 711, no., pp. 27-31., Registrované v: WOS
 12. [1.1] BIBI, Naheed - RATIER DE ARRUDA, Eduardo Guimaraes - DOMINGO, Alex - OLIVEIRA, Aline Alves - GALUPPO,

- Carolina - QUAN MANH PHUNG - ORRA, Naima Mohammed - BERON, Fanny - PAESANO, Andrea - PIERLOOT, Kristine - BARBOZA FORMIGA, Andre Luiz. Switching the Spin-Crossover Phenomenon by Ligand Design on Imidazole-Diazineiron(II) Complexes. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 23, pp. 14603-14616., Registrované v: WOS
13. [1.1] BICZYSKO, Malgorzata - BLOINO, Julien - PUZZARINI, Cristina. Computational challenges in Astrochemistry. In *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*. ISSN 1759-0876, 2018, vol. 8, no. 3, pp., Registrované v: WOS
14. [1.1] BICZYSKO, Malgorzata - KRUPA, Justyna - WIERZEJEWSKA, Maria. Theoretical studies of atmospheric molecular complexes interacting with NIR to UV light. In *FARADAY DISCUSSIONS*. ISSN 1359-6640, 2018, vol. 212, no., pp. 421-441., Registrované v: WOS
15. [1.1] BIENVENU, Alyssa V. - KNIZIA, Gerald. Efficient Treatment of Local Meta-generalized Gradient Density Functionals via Auxiliary Density Expansion: The Density Fitting J plus X Approximation. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 3, pp. 1297-1303., Registrované v: WOS
16. [1.1] BOGDANOVIC, Goran A. - OSTOJIC, Bojana D. - NOVAKOVIC, Sladjana B. Short Intramolecular O center dot center dot O Contact in Some o-Dialkoxybenzene Derivatives Generates Efficient Hydrogen Bonding Acceptor Area. In *CRYSTAL GROWTH & DESIGN*. ISSN 1528-7483, 2018, vol. 18, no. 3, pp. 1303-1314., Registrované v: WOS
17. [1.1] BOKHAN, Denis - TRUBNIKOV, Dmitrii N. - PERERA, Ajith - BARTLETT, Rodney J. Explicitly-correlated double ionization potentials and double electron attachment equation-of-motion coupled cluster methods. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 692, no., pp. 191-195., Registrované v: WOS
18. [1.1] BOKHAN, Denis - TRUBNIKOV, Dmitrii N. - PERERA, Ajith - BARTLETT, Rodney J. Spin-orbit splitted excited states using explicitly-correlated equation-of-motion coupled-cluster singles and doubles eigenvectors. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 698, no., pp. 171-175., Registrované v: WOS
19. [1.1] BOWMAN, Michael C. - BURKE, Alexandra D. - TURNEY, Justin M. - SCHAEFER, Henry F. Mechanisms of the Ethynyl Radical Reaction with Molecular Oxygen. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 49, pp. 9498-9511., Registrované v: WOS
20. [1.1] CABALEIRO-LAGO, Enrique M. - FERNANDEZ, Berta - RODRIGUEZ-OTERO, Jesus. Dissecting the Concave-Convex pi-pi Interaction in Corannulene and Sumanene Dimers: SAPT(DFT) Analysis and Performance of DFT Dispersion-Corrected Methods. In *JOURNAL OF COMPUTATIONAL CHEMISTRY*. ISSN 0192-8651, 2018, vol. 39, no. 2, pp. 93-104., Registrované v: WOS
21. [1.1] CABALEIRO-LAGO, Enrique M. - RODRIGUEZ-OTERO, Jesus. On the Nature of sigma-sigma, sigma-pi, and pi-pi Stacking in Extended Systems. In *ACS OMEGA*. ISSN 2470-1343, 2018, vol. 3, no. 8, pp. 9348-9359., Registrované v: WOS
22. [1.1] CERVINKA, Ctirad - BERAN, Gregory J. O. Ab initio prediction of the polymorph phase diagram for crystalline methanol. In *CHEMICAL SCIENCE*. ISSN 2041-6520, 2018, vol. 9, no. 20, pp. 4622-4629., Registrované v: WOS
23. [1.1] CHEDID, Julianna - FERRARA, Nashali M. - ESHUIS, Henk. Describing transition metal homogeneous catalysis using the random phase approximation. In *THEORETICAL CHEMISTRY ACCOUNTS*. ISSN 1432-881X, 2018, vol. 137, no. 11, pp., Registrované v: WOS
24. [1.1] CHEN, Guo P. - AGEE, Matthew M. - FURCHE, Filipp. Performance and Scope of Perturbative Corrections to Random-Phase Approximation Energies. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 11, pp. 5701-5714., Registrované v: WOS
25. [1.1] CHERAKI, Mohamed - AL-MOGREN, Muneerah Mogren - CHAMBAUD, Gilberte - FRANCISCO, Joseph S. - HOCHLAF, Majdi. Identification of Key Intermediates during the NO and H2S Crosstalk Signaling Pathways. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 11, pp. 2877-2883., Registrované v: WOS
26. [1.1] CHINNAMSETTY, Sambasiva Rao - GRIEBEL, Michael - HAMAEEKERS, Jan. AN ADAPTIVE MULTISCALE APPROACH FOR ELECTRONIC STRUCTURE METHODS. In *MULTISCALE MODELING & SIMULATION*. ISSN 1540-3459, 2018, vol. 16, no. 2, pp. 752-776., Registrované v: WOS
27. [1.1] CHOJECKI, Michal - YOURDKHANI, Sirous - RUTKOWSKA-ZBIK, Dorota - KORONA, Tatiana. Stability of endo- and exohedral complexes of all-boron fullerene B-40. In *COMPUTATIONAL AND THEORETICAL CHEMISTRY*. ISSN 2210-271X, 2018, vol. 1133, no., pp. 7-17., Registrované v: WOS
28. [1.1] CLAUDINO, Daniel - BARTLETT, Rodney J. Coupled-cluster based basis sets for valence correlation calculations. New primitives, frozen atomic natural orbitals, and basis sets from double to hexuple zeta for atoms H, He, and B-Ne. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 6, pp., Registrované v: WOS
29. [1.1] DIAZ-TINOCO, Manuel - CORZO, H. H. - ORTIZ, J. V. Electron Propagator Methods for Vertical Electron Detachment Energies of Anions: Benchmarks and Case Studies. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 11, pp. 5881-5895., Registrované v: WOS
30. [1.1] DIXIT, Anant - CLAUDOT, Julien - GOULD, Tim - LEBEGUE, Sebastien - ROCCA, Dario. Methods for converging correlation energies within the dielectric matrix formalism. In *PHYSICAL REVIEW B*. ISSN 2469-9950, 2018, vol. 97, no. 11, pp., Registrované v: WOS
31. [1.1] DUTTA, Narendra Nath - PATKOWSKI, Konrad. Improving "Silver-Standard" Benchmark Interaction Energies with Bond Functions. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 6, pp. 3053-3070., Registrované v: WOS
32. [1.1] FABER, Rasmus - SAUER, Stephan P. A. On the convergence of the ccJ-pVXZ and pcJ-n basis sets in CCSD calculations of nuclear spin-spin coupling constants: some difficult cases. In *THEORETICAL CHEMISTRY ACCOUNTS*. ISSN 1432-881X, 2018, vol. 137, no. 3, pp., Registrované v: WOS
33. [1.1] FELLER, David - DAVIDSON, Ernest R. A theoretical study of the adiabatic and vertical ionization potentials of water. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 23, pp., Registrované v: WOS
34. [1.1] FORTENBERRY, Ryan C. - NOVAK, Carlie M. - LEE, Timothy J. Rovibrational analysis of c-SiC2H2: Further evidence for out-of-plane bending issues in correlated methods. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 2, pp., Registrované v: WOS
35. [1.1] FRANKE, Peter R. - DOUBERLY, Gary E. Rotamers of Isoprene: Infrared Spectroscopy in Helium Droplets and Ab Initio

- Thermochemistry. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 1, pp. 148-158., Registrované v: WOS*
36. [1.1] GAJDA, Lukasz - KUPKA, Teobald - BRODA, Malgorzata A. - LESZCZYNSKA, Malgorzata - EJSMONT, Krzysztof. Method and basis set dependence of the NICS indexes of aromaticity for benzene. In *MAGNETIC RESONANCE IN CHEMISTRY. ISSN 0749-1581, 2018, vol. 56, no. 4, pp. 265-275., Registrované v: WOS*
37. [1.1] GAWRILOW, Maxim - BECKERS, Helmut - RIEDEL, Sebastian - CHENG, Lan. Matrix-Isolation and Quantum-Chemical Analysis of the $\text{ITC}&\text{ITv}&\text{IT}$ Conformer of XeF_6 , XeOF_4 , and Their Acetonitrile Adducts. In *JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 1, pp. 119-129., Registrované v: WOS*
38. [1.1] GREIN, Friedrich. Ab initio studies of the van der Waals complex $\text{CH}_4\text{-O-2 center dot CH center dot center dot center dot O}$ and $\text{CX center dot center dot center dot O}$ interactions in halomethane $\text{XnCH}_4\text{-n-O-2 complexes}$ ($\text{X} = \text{F, Cl; n} = 1, 2, 3$). In *THEORETICAL CHEMISTRY ACCOUNTS. ISSN 1432-881X, 2018, vol. 137, no. 5, pp., Registrované v: WOS*
39. [1.1] HOOBLER, Preston R. - TURNEY, Justin M. - AGARWAL, Jay - SCHAEFER, Henry F. Fundamental Vibrational Analyses of the HCN Monomer, Dimer and Associated Isotopologues. In *CHEMPHYSICHEM. ISSN 1439-4235, 2018, vol. 19, no. 23, pp. 3257-3265., Registrované v: WOS*
40. [1.1] HOWARD, J. Coleman - SOWNDARYA, Shree S. V. - ANSARI, Imaad M. - MACH, Taylor J. - BARANOWSKA-LACZKOWSKA, Angelika - CRAWFORD, T. Daniel. Performance of Property-Optimized Basis Sets for Optical Rotation with Coupled Cluster Theory. In *JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 28, pp. 5962-5969., Registrované v: WOS*
41. [1.1] JAVADIAN, Soheila - KHOSRAVIAN, Mahnaz. Revealing Factors Governing Self-Assembly Morphology of Fatty Acid on Graphene Synthesized by Surfactant-Assisted LPE: A Joint MD, SAPT(DFT), and Experimental Study. In *JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, 2018, vol. 122, no. 37, pp. 21387-21400., Registrované v: WOS*
42. [1.1] JERABEK, Paul - SCHWERTDFEGGER, Peter - NAGLE, Jeffrey K. Static dipole polarizability of palladium from relativistic coupled-cluster theory. In *PHYSICAL REVIEW A. ISSN 2469-9926, 2018, vol. 98, no. 1, pp., Registrované v: WOS*
43. [1.1] JORGENSEN, Kameron R. - CADENA, Melissa. Theoretical study of bromine halocarbons: Accurate enthalpies of formation. In *COMPUTATIONAL AND THEORETICAL CHEMISTRY. ISSN 2210-271X, 2018, vol. 1141, no., pp. 66-73., Registrované v: WOS*
44. [1.1] KALAI, Cairedine - TOULOUSE, Julien. A general range-separated double-hybrid density-functional theory. In *JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 16, pp., Registrované v: WOS*
45. [1.1] KARIR, Gimny - KUMAR, Gaurav - KAR, Bishnu Prasad - VISWANATHAN, K. S. Multiple Hydrogen Bond Tethers for Grazing Formic Acid in Its Complexes with Phenylacetylene. In *JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 8, pp. 2046-2059., Registrované v: WOS*
46. [1.1] KIM, Dong Yeon - YANG, D. ChangMo - MADRIDAJOS, Jenica Marie L. - HAJIBABAEI, Amir - BAIG, Chunggi - KIM, Kwang S. Anisotropic and amphoteric characteristics of diverse carbenes. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS. ISSN 1463-9076, 2018, vol. 20, no. 20, pp. 13722-13733., Registrované v: WOS*
47. [1.1] KIRSCHNER, Karl N. - HEIDEN, Wolfgang - REITH, Dirk. Small Alcohols Revisited: CCSD(T) Relative Potential Energies for the Minima, First- and Second-Order Saddle Points, and Torsion-Coupled Surfaces. In *ACS OMEGA. ISSN 2470-1343, 2018, vol. 3, no. 1, pp. 419-432., Registrované v: WOS*
48. [1.1] KRASNOSHCHEKOV, Sergey - LAPTEV, Vladimir B. - GAINULLIN, Ivan K. Absolute IR vibrational band intensities of hexafluoroacetone: Comparison of experiment and anharmonic ab initio calculation using the second-order operator canonical Van Vleck perturbation theory. In *JOURNAL OF QUANTITATIVE SPECTROSCOPY & RADIATIVE TRANSFER. ISSN 0022-4073, 2018, vol. 217, no., pp. 243-252., Registrované v: WOS*
49. [1.1] KRASNOSHCHEKOV, Sergey V. - SCHUTSKI, Roman S. - CRAIG, Norman C. - SIBAEV, Marat - CRITTENDEN, Deborah L. Comparing the accuracy of perturbative and variational calculations for predicting fundamental vibrational frequencies of dihalomethanes. In *JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 8, pp., Registrované v: WOS*
50. [1.1] KUPKA, Teobald - BUCZEK, Aneta - BRODA, Malgorzata A. - GAJDA, Lukasz - IGNASIAK, Monika. Convergence of nuclear magnetic shieldings and one-bond $\langle 1J(\text{BH})\text{-B-11-H-1} \rangle$ indirect spin-spin coupling constants in small boron molecules. In *MAGNETIC RESONANCE IN CHEMISTRY. ISSN 0749-1581, 2018, vol. 56, no. 5, pp. 338-351., Registrované v: WOS*
51. [1.1] LABANC, Daniel - SULKA, Martin - PITONAK, Michal - CERNUSAK, Ivan - URBAN, Miroslav - NEOGRADY, Pavel. Benchmark CCSD(T) and DFT study of binding energies in Be7-12 : in search of reliable DFT functional for beryllium clusters. In *MOLECULAR PHYSICS. ISSN 0026-8976, 2018, vol. 116, no. 10, pp. 1259-1274., Registrované v: WOS*
52. [1.1] LAHM, Mitchell E. - HOOBLER, Preston R. - TURNEY, Justin M. - PETERSON, Kirk A. - SCHAEFER, Henry F. The bismuth tetramer Bi_4 : the $\nu(3)$ key to experimental observation. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS. ISSN 1463-9076, 2018, vol. 20, no. 34, pp. 21881-21889., Registrované v: WOS*
53. [1.1] LAM, Chow-Shing - LAU, Kai-Chung - NG, Cheuk-Yiu. High-level ab initio predictions for the ionisation energy, bond dissociation energies and heats of formation of zirconium oxide and its cation (ZrO/ZrO^+). In *MOLECULAR PHYSICS. ISSN 0026-8976, 2018, vol. 116, no. 19-20, pp. 2709-2718., Registrované v: WOS*
54. [1.1] LEE, Joonho - HEAD-GORDON, Martin. Regularized Orbital-Optimized Second-Order Moller-Plesset Perturbation Theory: A Reliable Fifth-Order-Scaling Electron Correlation Model with Orbital Energy Dependent Regularizers. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 10, pp. 5203-5219., Registrované v: WOS*
55. [1.1] LI, M. W. - ZIMMERMAN, P. M. Stepwise basis set selection. In *JOURNAL OF COMPUTATIONAL CHEMISTRY. ISSN 0192-8651, 2018, vol. 39, no. 26, pp. 2153-2162., Registrované v: WOS*
56. [1.1] LIU, Junzi - SHEN, Yue - ASTHANA, Ayush - CHENG, Lan. Two-component relativistic coupled-cluster methods using mean-field spin-orbit integrals. In *JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 3, pp., Registrované v: WOS*
57. [1.1] LUTZ, Jesse J. - DUAN, Xiaofeng F. - RANASINGHE, Duminda S. - JIN, Yifan - MARGRAF, Johannes T. - PERERA, Ajith - BURGGRAF, Larry W. - BARTLETT, Rodney J. Valence and charge-transfer optical properties for some SinCm ($m, n \leq 12$) clusters: Comparing TD-DFT, complete-basis-limit EOMCC, and benchmarks from spectroscopy. In *JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 17, pp., Registrované v: WOS*

58. [1.1] MAGOULAS, Ilias - BAUMAN, Nicholas P. - SHEN, Jun - PIECUCH, Piotr. Application of the CC(P;Q) Hierarchy of Coupled Cluster Methods to the Beryllium Dimer. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 5, pp. 1350-1368., Registrované v: WOS
59. [1.1] MALENOV, Dusan P. - ANTONIJEVIC, Ivana S. - HALL, Michael B. - ZARIC, Snezana D. Stacking of cyclopentadienyl organometallic sandwich and half-sandwich compounds. Strong interactions of sandwiches at large offsets. In *CRYSTENGCOMM*. ISSN 1466-8033, 2018, vol. 20, no. 31, pp. 4506-4514., Registrované v: WOS
60. [1.1] MARTIN, Jan M. L. A Simple 'Range Extender' for Basis Set Extrapolation Methods for MP2 and Coupled Cluster Correlation Energies. In *INTERNATIONAL CONFERENCE OF COMPUTATIONAL METHODS IN SCIENCES AND ENGINEERING 2018 (ICCMSE-2018)*. ISSN 0094-243X, 2018, vol. 2040, no., pp., Registrované v: WOS
61. [1.1] MCDONALD, David C. - WAGNER, J. Philipp - DUNCAN, Michael A. Mid/near infrared spectroscopy of the H₂Cl⁺ Ar cation complex compared to the predictions of anharmonic theory. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 691, no., pp. 51-55., Registrované v: WOS
62. [1.1] MCKINLEY, Jessica L. - BERAN, Gregory J. O. Identifying pragmatic quasi-harmonic electronic structure approaches for modeling molecular crystal thermal expansion. In *FARADAY DISCUSSIONS*. ISSN 1359-6640, 2018, vol. 211, no., pp. 181-207., Registrované v: WOS
63. [1.1] MEDEIROS, D. J. - BLITZ, M. A. - JAMES, L. - SPEAK, T. H. - SEAKINS, P. W. Kinetics of the Reaction of OH with Isoprene over a Wide Range of Temperature and Pressure Including Direct Observation of Equilibrium with the OH Adducts. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 37, pp. 7239-7255., Registrované v: WOS
64. [1.1] MEITEI, Oinam Romesh - HESSELMANN, Andreas. Geometry optimizations with the incremental molecular fragmentation method. In *JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY*. ISSN 0219-6336, 2018, vol. 17, no. 5, pp., Registrované v: WOS
65. [1.1] MELLI, Alessio - MELOSSO, Mattia - TASINATO, Nicola - BOSI, Giulio - SPADA, Lorenzo - BLOINO, Julien - MENDOLICCHIO, Marco - DORE, Luca - BARONE, Vincenzo - PUZZARINI, Cristina. Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection. In *ASTROPHYSICAL JOURNAL*. ISSN 0004-637X, 2018, vol. 855, no. 2, pp., Registrované v: WOS
66. [1.1] MISHRA, Brijesh Kumar - VENKATNARAYAN, Ramanathan. Substituents' influence on the C-H center dot center dot center dot pi interaction in the T-shaped benzene dimer. In *THEORETICAL CHEMISTRY ACCOUNTS*. ISSN 1432-881X, 2018, vol. 137, no. 5, pp., Registrované v: WOS
67. [1.1] MISIEWICZ, Jonathon P. - ELLIOTT, Sarah N. - MOORE, Kevin B. - SCHAEFER, Henry F. Re-examining ammonia addition to the Criegee intermediate: converging to chemical accuracy. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 11, pp. 7479-7491., Registrované v: WOS
68. [1.1] MISIEWICZ, Jonathon P. - NOONAN, Julia A. - TURNEY, Justin M. - SCHAEFER, Henry F. The non-covalently bound SO center dot center dot center dot H₂O system, including an interpretation of the differences between SO center dot center dot center dot H₂O and O-2 center dot center dot center dot H₂O. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 45, pp. 28840-28847., Registrované v: WOS
69. [1.1] MORGAN, W. James - HUANG, Xinchuan - SCHAEFER, Henry F. - LEE, Timothy J. Astrophysical sulfur in diffuse and dark clouds: The fundamental vibrational frequencies and spectroscopic constants of hydrogen sulfide cation (H₂S⁺). In *MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY*. ISSN 0035-8711, 2018, vol. 480, no. 3, pp. 3483-3490., Registrované v: WOS
70. [1.1] MORGAN, W. James - MATTHEWS, Devin A. - RINGHOLM, Magnus - AGARWAL, Jay - GONG, Justin Z. - RUUD, Kenneth - ALLEN, Wesley D. - STANTON, John F. - SCHAEFER, Henry F. Geometric Energy Derivatives at the Complete Basis Set Limit: Application to the Equilibrium Structure and Molecular Force Field of Formaldehyde. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 3, pp. 1333-1350., Registrované v: WOS
71. [1.1] MOTTA, Mario - ZHANG, Shiwei. Ab initio computations of molecular systems by the auxiliary-field quantum Monte Carlo method. In *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*. ISSN 1759-0876, 2018, vol. 8, no. 5, pp., Registrované v: WOS
72. [1.1] NAGY, Peter R. - SAMU, Gyula - KALLAY, Mihaly. Optimization of the Linear-Scaling Local Natural Orbital CCSD(T) Method: Improved Algorithm and Benchmark Applications. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 8, pp. 4193-4215., Registrované v: WOS
73. [1.1] OBENCHAIN, Daniel A. - SPADA, Lorenzo - ALESSANDRINI, Silvia - RAMPINO, Sergio - HERBERS, Sven - TASINATO, Nicola - MENDOLICCHIO, Marco - KRAUS, Peter - GAUSS, Jurgen - PUZZARINI, Cristina - GRABOW, Jens-Uwe - BARONE, Vincenzo. Unveiling the Sulfur-Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. In *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*. ISSN 1433-7851, 2018, vol. 57, no. 48, pp. 15822-15826., Registrované v: WOS
74. [1.1] OSTOJIC, B. D. - SCHWERTFEGER, P. - DORDEVIC, D. S. Modeling the hydrogen sulfide binding to heme. In *JOURNAL OF INORGANIC BIOCHEMISTRY*. ISSN 0162-0134, 2018, vol. 184, no., pp. 108-114., Registrované v: WOS
75. [1.1] OTKJAER, Rasmus V. - JAKOBSEN, Helene H. - TRAM, Camilla Mia - KJAERGAARD, Henrik G. Calculated Hydrogen Shift Rate Constants in Substituted Alkyl Peroxy Radicals. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 43, pp. 8665-8673., Registrované v: WOS
76. [1.1] POSADA, Edwin - MONCADA, Felix - REYES, Andres. The any particle molecular orbital grid-based Hartree-Fock (APMO-GBHF) approach. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 8, pp., Registrované v: WOS
77. [1.1] PRUDENZANO, D. - LAAS, J. - BIZZOCCHI, L. - LATTANZI, V - ENDRES, C. - GIULIANO, B. M. - SPEZZANO, S. - PALUMBO, M. E. - CASELLI, P. Accurate millimetre and submillimetre rest frequencies for cis- and trans-dithioformic acid, HCSSH. In *ASTRONOMY & ASTROPHYSICS*. ISSN 1432-0746, 2018, vol. 612, no., pp., Registrované v: WOS
78. [1.1] QUAN MANH PHUNG - FELDT, Milica - HARVEY, Jeremy N. - PIERLOOT, Kristine. Toward Highly Accurate Spin State Energetics in First-Row Transition Metal Complexes: A Combined CASPT2/CC Approach. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 5, pp. 2446-2455., Registrované v: WOS
79. [1.1] QUAN MANH PHUNG - PIERLOOT, Kristine. The dioxygen adducts of iron and manganese porphyrins: electronic

- structure and binding energy. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 25, pp. 17009-17019., Registrované v: WOS
80. [1.1] REDONDO, Pilar - LARGO, Antonio - BARRIENTOS, Carmen. Structure and spectroscopic properties of imine acetaldehyde: a possible interstellar molecule. In *MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY*. ISSN 0035-8711, 2018, vol. 478, no. 3, pp. 3042-3048., Registrované v: WOS
81. [1.1] REDONDO, Pilar - RAYON, Victor M. - BARRIENTOS, Carmen - LARGO, Antonio. Structural Trends in Monoboronil Compounds: Analysis of the Interaction of Second-Row Elements with BO. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 1, pp. 398-409., Registrované v: WOS
82. [1.1] REZAC, Jan - BIM, Daniel - GUTTEN, Ondrej - RULISEK, Lubomir. Toward Accurate Conformational Energies of Smaller Peptides and Medium-Sized Macrocycles: MPCONF196 Benchmark Energy Data Set. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 3, pp. 1254-1266., Registrované v: WOS
83. [1.1] REZAC, Jan - GREENWELL, Chandler - BERAN, Gregory J. O. Accurate Noncovalent Interactions via Dispersion-Corrected Second-Order Moller-Plesset Perturbation Theory. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 9, pp. 4711-4721., Registrované v: WOS
84. [1.1] RICHARD, Ryan M. - BAKR, Brandon W. - SHERRILL, C. David. Understanding the Many-Body Basis Set Superposition Error: Beyond Boys and Bernardi. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 5, pp. 2386-2400., Registrované v: WOS
85. [1.1] RYBICKI, Marcin - SAUER, Joachim. Ab Initio Prediction of Proton Exchange Barriers for Alkanes at Bronsted Sites of Zeolite H-MFI. In *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*. ISSN 0002-7863, 2018, vol. 140, no. 51, pp. 18151-18161., Registrované v: WOS
86. [1.1] SHAHBAZ, Muhammad - SZALEWICZ, Krzysztof. Do Semilocal Density-Functional Approximations Recover Dispersion Energies at Small Intermonomer Separations? In *PHYSICAL REVIEW LETTERS*. ISSN 0031-9007, 2018, vol. 121, no. 11, pp., Registrované v: WOS
87. [1.1] SHEE, James - ARTHUR, Evan J. - ZHANG, Shiwei - REICHMAN, David R. - FRIESNER, Richard A. Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 8, pp. 4109-4121., Registrované v: WOS
88. [1.1] SHIBL, Mohamed F. - MONCHO, Salvador - BROTHERS, Edward N. What Happens Without Nickel? Cyclization Reactions of Ethylene with Ethanedithial and Related Molecules. In *JOURNAL OF COMPUTATIONAL CHEMISTRY*. ISSN 0192-8651, 2018, vol. 39, no. 18, pp. 1158-1167., Registrované v: WOS
89. [1.1] SMIGAR, Szymon - GRABOWSKI, Ireneusz. Spin-Component-Scaled Delta MP2 Parametrization: Toward a Simple and Reliable Method for Ionization Energies. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 9, pp. 4780-4790., Registrované v: WOS
90. [1.1] SZORI, Milan - GIRI, Binod Raj - WANG, Zhandong - DAWOOD, Alaaeldin E. - VISKOLCZ, Bela - FAROOQ, Aamir. Glycerol carbonate as a fuel additive for a sustainable future. In *SUSTAINABLE ENERGY & FUELS*. ISSN 2398-4902, 2018, vol. 2, no. 10, pp. 2171-2178., Registrované v: WOS
91. [1.1] TARUMI, Moto - NAKAI, Hiromi. Quantum chemical approach for condensed-phase thermochemistry (V): Development of rigid-body type harmonic solvation model. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 700, no., pp. 149-155., Registrované v: WOS
92. [1.1] TASI, Domonkos Attila - CSONTOS, Jozsef - NAGY, Balazs - KONYA, Zoltan - TASI, Gyula. Comment on "Causation or only correlation? Application of causal inference graphs for evaluating causality in nano-QSAR models" by N. Sizochenko, A. Gajewicz, J. Leszczynski and T. Puzyn, *Nanoscale*, 2016, 8, 7203. In *NANOSCALE*. ISSN 2040-3364, 2018, vol. 10, no. 44, pp. 20863-20866., Registrované v: WOS
93. [1.1] TECMER, Pawel - GONZALEZ-ESPINOZA, Cristina E. Electron correlation effects of the ThO and ThS molecules in the spinor basis. A relativistic coupled cluster study of ground and excited states properties. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 36, pp. 23424-23432., Registrované v: WOS
94. [1.1] TOBIAS, Roland - CSASZAR, Attila G. - GYEVI-NAGY, Laszlo - TASI, Gyula. Definitive thermochemistry and kinetics of the interconversions among conformers of n-butane and n-pentane. In *JOURNAL OF COMPUTATIONAL CHEMISTRY*. ISSN 0192-8651, 2018, vol. 39, no. 8, pp. 424-437., Registrované v: WOS
95. [1.1] TRABELSI, Tarek - AL MOGREN, Muneerah Mogren - HOCHLAF, Majdi - FRANCISCO, Joseph S. Electronic and spectroscopic characterizations of SNP isomers. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 5, pp., Registrované v: WOS
96. [1.1] TRABELSI, Tarek - AL-MOGREN, Muneerah Mogren - HOCHLAF, Majdi - FRANCISCO, Joseph S. Mechanistic study of the photoexcitation, photoconversion, and photodissociation of CS₂. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 6, pp., Registrované v: WOS
97. [1.1] TRABELSI, Tarek - HOCHLAF, Majdi - FRANCISCO, Joseph S. Toward the detection of the triatomic negative ion SPN⁻: Spectroscopy and potential energy surfaces. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 16, pp., Registrované v: WOS
98. [1.1] UNAL, Asli - BOZKAYA, Ugur. Anionic water pentamer and hexamer clusters: An extensive study of structures and energetics. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 12, pp., Registrované v: WOS
99. [1.1] VARANDAS, A. J. C. CBS extrapolation in electronic structure pushed to the end: a revival of minimal and sub-minimal basis sets. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 34, pp. 22084-22098., Registrované v: WOS
100. [1.1] VARANDAS, Antonio J. C. Straightening the Hierarchical Staircase for Basis Set Extrapolations: A Low-Cost Approach to High-Accuracy Computational Chemistry. In *ANNUAL REVIEW OF PHYSICAL CHEMISTRY*, VOL 69. ISSN 0066-426X, 2018, vol. 69, no., pp. 177-203., Registrované v: WOS
101. [1.1] VERMA, Kanupriya - VISWANATHAN, K. S. "A Tale of Two Structures": The Stacks and Ts of Borazine and Benzene Hetero and Homo Dimers. In *CHEMISTRYSELECT*. ISSN 2365-6549, 2018, vol. 3, no. 3, pp. 864-873., Registrované v: WOS

102. [1.1] VICHETTI, R. M. - DA SILVA, A. B. F. - HAIDUKE, R. L. A. Providing theoretical data for detection of four formamidic acid isomers in astrophysical media. In *MOLECULAR ASTROPHYSICS*. ISSN 2405-6758, 2018, vol. 10, no., pp. 1-10., Registrované v: WOS
103. [1.1] VINDEL-ZANDBERGEN, Patricia - JIANG, Ji - LEWERENZ, Marius - MEIER, Christoph - BARRANCO, Manuel - PI, Marti - HALBERSTADT, Nadine. Impulsive alignment of (4)He-CH₃I: A theoretical study. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 12, pp., Registrované v: WOS
104. [1.1] WAGNER, J. Philipp - MCDONALD, David C. - DUNCAN, Michael A. An Argon-Oxygen Covalent Bond in the ArOH⁺ Molecular Ion. In *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*. ISSN 1433-7851, 2018, vol. 57, no. 18, pp. 5081-5085., Registrované v: WOS
105. [1.1] WEIDMAN, Jared D. - ALLEN, Ryan T. - MOORE, Kevin B. - SCHAEFER, Henry F. High level theoretical characterization of the vinyoxy radical (center dot CH₂CHO) + O-2 reaction. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 18, pp., Registrované v: WOS
106. [1.1] WICK, Christian R. - SMITH, David M. Modeling the Reactions Catalyzed by Coenzyme B-12 Dependent Enzymes: Accuracy and Cost-Quality Balance. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 6, pp. 1747-1755., Registrované v: WOS
107. [1.1] WIENS, Avery E. - COPAN, Andreas V. - ROSSOMME, Elliot C. - AROEIRA, Gustavo J. R. - BERNSTEIN, Olivia M. - AGARWAL, Jay - SCHAEFER, Henry F. Reinterpreting the infrared spectrum of H plus HCN: Methylene amidogen radical and its coproducts. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 1, pp., Registrované v: WOS
108. [1.1] WONG, Z. C. - FAN, W. Y. - CHWEE, T. S. Computational modelling of singlet excitation energy transfer: a DFT/TD-DFT study of the ground and excited state properties of a syn bimane dimer system using non-empirically tuned range-separated functionals. In *NEW JOURNAL OF CHEMISTRY*. ISSN 1144-0546, 2018, vol. 42, no. 16, pp. 13732-13743., Registrované v: WOS
109. [1.1] WU, Qiyang - SU, He - WANG, Hongyan - WANG, Hui. Ab initio calculations, structure, NBO and NCI analyses of X-H...pi interactions. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 693, no., pp. 202-209., Registrované v: WOS
110. [1.1] YANG, Mino. What Function Is Optimal for CCSD(T) Complete Basis Extrapolation for OH Stretching Potential of Water Molecules? In *BULLETIN OF THE KOREAN CHEMICAL SOCIETY*. ISSN 1229-5949, 2018, vol. 39, no. 1, pp. 52-57., Registrované v: WOS
111. [1.1] YOURDKHANI, Sirous - CHOJECKI, Michal - KORONA, Tatiana. Interaction of Non-polarizable Cations with Azaborine Isomers and Their Mono-Substituted Derivatives: Position, Induction, and Non-Classical Effects Matter. In *CHEMPHYSICHEM*. ISSN 1439-4235, 2018, vol. 19, no. 22, pp. 3092-3106., Registrované v: WOS
- ADCA135 HESABI, Z. Razavi - HAGHIGHATZADEH, M. - MAZAHARI, Mehdi - GALUSEK, Dušan - SADRNEZHAAD, S.K. Suppression of grain growth in sub-micrometer alumina via two-step sintering method. In *Journal of the European Ceramic Society*, 2009, vol. 29, no. 8, p. 1371-1377. (2008: 1.580 - IF, karentované - CCC). (2009 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.
- Citácie:
1. [1.1] CHEN, Feng - YAN, Zhiqiao. Preparation of 3Y-TZP Nanoceramics by a Modified Two-Step Sintering with Ultrahigh Heating and Cooling Rates. In *ADVANCED FUNCTIONAL MATERIALS (CMC 2017)*, 2018, vol., no., pp. 651-659., Registrované v: WOS
2. [1.1] LI, Lu - PU, Sanxu - LIU, Yuhang - ZHAO, Libin - MA, Ji - LI, Jiangong. High-purity disperse alpha-Al₂O₃ nanoparticles synthesized by high-energy ball milling. In *ADVANCED POWDER TECHNOLOGY*. ISSN 0921-8831, 2018, vol. 29, no. 9, pp. 2194-2203., Registrované v: WOS
3. [1.1] LIU, Zhen - LU, Teng - YE, Jiaming - WANG, Genshui - DONG, Xianlin - WITHERS, Ray - LIU, Yun. Antiferroelectrics for Energy Storage Applications: a Review. In *ADVANCED MATERIALS TECHNOLOGIES*. ISSN 2365-709X, 2018, vol. 3, no. 9, pp., Registrované v: WOS
4. [1.1] OJAIMI, Christiane Lago - FERREIRA, Julieta Adriana - DOS SANTOS, Fabio Andre - CHINELATTO, Adilson Luiz - DE JESUS AGNOLON PALLONE, Eliria Maria - ANTONIO CHINELATTO, Adriana Scoton. Mechanical characterisation and hydrothermal degradation of Al₂O₃-15 % vol ZrO₂ nanocomposites consolidated by two-step sintering. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 14, pp. 16128-16136., Registrované v: WOS
5. [1.1] TAVANGARIAN, Fariborz - FAHAMI, Abbas - LI, Guoqiang - KAZEMI, Mohammadhassan - FORGHANI, Anoosha. Structural characterization and strengthening mechanism of forsterite nanostructured scaffolds synthesized by multistep sintering method. In *JOURNAL OF MATERIALS SCIENCE & TECHNOLOGY*. ISSN 1005-0302, 2018, vol. 34, no. 12, pp. 2263-2270., Registrované v: WOS
- ADCA136 HNATKO, Miroslav - GALUSEK, Dušan - ŠAJGALÍK, Pavol. Low-cost preparation of Si₃N₄-SiC micro/nano composites by in-situ carbothermal reduction of silica in silicon nitride matrix. In *Journal of the European Ceramic Society*, 2004, vol. 24, no. 2, p. 189-195. ISSN 0955-2219.
- Citácie:
1. [1.1] BABU, Ganesh T. - BHUVANESWARI, S. - DEVASIA, Renjith. Synthesis and ceramic conversion of novel silazane modified phenol formaldehyde resin. In *MATERIALS CHEMISTRY AND PHYSICS*. ISSN 0254-0584, 2018, vol. 212, no., pp. 175-186., Registrované v: WOS
- ADCA137 HOLEŠOVÁ, Sylva - VALÁŠKOVÁ, Marta - HLAVÁČ, Dominik - MADEJOVÁ, Jana - SAMLÍKOVÁ, Magda - TOKARSKÝ, Jonáš - PAZDZIARA, Erich. Antibacterial kaolinite/urea/chlorhexidine nanocomposites: Experiment and molecular modelling. In *Applied Surface Science*, 2014, vol. 305, p. 783-791. (2013: 2.538 - IF, 0.965 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 0169-4332.
- Citácie:
1. [1.1] LOBATO-AGUILAR, H. - URIBE-CALDERON, J. A. - HERRERA-KAO, W. - DUARTE-ARANDA, S. - BAAS-LOPEZ, J. M. - ESCOBAR-MORALES, B. - CAUCH-RODRIGUEZ, J. - CERVANTES-UC, J. M. Synthesis, characterization and chlorhexidine release from either montmorillonite or palygorskite modified organoclays for antibacterial applications. In *JOURNAL OF DRUG DELIVERY SCIENCE AND TECHNOLOGY*. ISSN 1773-2247, 2018, vol. 46, no., pp. 452-460.,

Registrované v: WOS

2. [1.1] ZHANG, Zhifang - WANG, Wenbo - KANG, Yuru - WANG, Qin - WANG, Aiqin. Structure evolution of brick-red palygorskite induced by hydroxylammonium chloride. In *POWDER TECHNOLOGY*. ISSN 0032-5910, 2018, vol. 327, no., pp. 246-254., Registrované v: WOS

ADCA138 HONTY, Miroslav - DE CRAEN, Mieke - WANG, Lian - MADEJOVÁ, Jana - CZÍMEROVÁ, Adriana - PENTRÁK, Martin - STRÍČEK, Igor - VAN GEET, Maarten. The effect of high pH alkaline solutions on the mineral stability of the Boom Clay - Batch experiments at 60 °C. In *Applied Geochemistry*, 2010, vol. 25, no. 6, p. 825-840. (2009: 1.961 - IF, karentované - CCC). (2010 - Current Contents). ISSN 0883-2927.

Citácie:

1. [1.1] GERAMIAN, Mirjavad - IVEY, Douglas G. - LIU, Qi - ETSELL, Thomas H. Characterization of four petrologic end members from Alberta oil sands and comparison between different mines and sampling times. In *CANADIAN JOURNAL OF CHEMICAL ENGINEERING*. ISSN 0008-4034, 2018, vol. 96, no. 1, pp. 49-61., Registrované v: WOS
2. [1.1] ZHANG, Tingting - ZOU, Jing - WANG, Baomin - WU, Zhenlin - JIA, Yuan - CHEESEMAN, Christopher R. Characterization of Magnesium Silicate Hydrate (MSH) Gel Formed by Reacting MgO and Silica Fume. In *MATERIALS*. ISSN 1996-1944, 2018, vol. 11, no. 6, pp., Registrované v: WOS

ADCA139 HRACHOVÁ, Jana - KOMADEL, Peter - JOCHEC MOŠKOVÁ, Daniela - KRAJČI, Juraj - JANIGOVÁ, Ivica - ŠLOUF, Miroslav - CHODÁK, Ivan. Properties of organo-clay/natural rubber nanocomposites: Effects of organophilic modifiers. In *Journal of Applied Polymer Science*, 2013, vol. 127, p. 3447 - 3455. (2012: 1.395 - IF, 0.658 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 0021-8995.

Citácie:

1. [1.1] HU, L. - PEPIN, K. - BEBIN, P. - LECLAIR, E. - COLAS, F. - VUILLAUME, P.Y. Fluorohectorite/LDPE nanocomposites: The role of organomodifiers and compatibilizer. In *CANADIAN JOURNAL OF CHEMICAL ENGINEERING*. ISSN 0008-4034, JUL 2018, vol. 96, no. 7, p. 1510-1517., Registrované v: WOS
2. [1.1] JAYARAJ, S. - EGODAGE, S.M. - WALPALAGE, S. New approach for preparation of dry natural rubber nanocomposites through acid-free co-coagulation: Effect of organoclay content. In *JOURNAL OF APPLIED POLYMER SCIENCE*. ISSN 0021-8995, JUN 20 2018, vol. 135, no. 28., Registrované v: WOS

ADCA140 HRACHOVÁ, Jana - KOMADEL, Peter - JANIGOVÁ, Ivica - ŠLOUF, Miroslav - CHODÁK, Ivan. Properties of rubber filled with montmorillonite with various surface modifications. In *Polymers for Advanced Technologies*, 2012, vol. 23, p. 1414 - 1421. (2011: 2.007 - IF, 0.835 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 1042-7147.

Citácie:

1. [1.1] BIZOVSKA, V. - JANKOVIC, L. - MADEJOVA, J. Montmorillonite modified with unconventional surfactants from the series of octylammonium-based cations: Structural characterization and hydration properties. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, JUN 15 2018, vol. 158, p. 102-112., Registrované v: WOS

ADCA141 HRACHOVÁ, Jana - KOMADEL, Peter - CHODÁK, Ivan. Effect of montmorillonite modification on mechanical properties of vulcanized natural rubber composites. In *Journal of Materials Science*, 2008, vol. 43, no. 6, p. 2012-2017. (2007: 1.081 - IF, karentované - CCC). (2008 - Current Contents). ISSN 0022-2461.

Citácie:

1. [1.1] CAO, J. - WEN, N. - ZHENG, Y.Y. The preparation of calcium pimelate modified OMMT from natural Camontmorillonite and its application as beta-nucleating agent for polypropylene. In *POLYMER TESTING*. ISSN 0142-9418, FEB 2018, vol. 65, p. 352-359., Registrované v: WOS
2. [1.1] MANDAL, N. - DATTA, S.C. - MANJAIAH, K.M. - DWIVEDI, B.S. - KUMAR, R. - AGGARWAL, P. Zincated Nanoclay Polymer Composites (ZNCPCs): Synthesis, Characterization, Biodegradation and Controlled Release Behaviour in Soil. In *POLYMER-PLASTICS TECHNOLOGY AND ENGINEERING*. ISSN 0360-2559, 2018, vol. 57, no. 17, p. 1760-1770., Registrované v: WOS
3. [1.1] MANDAL, N. - DATTA, S.C. - MANJAIAH, K.M. - DWIVEDI, B.S. - NAIN, L. - KUMAR, R. - AGGARWAL, P. Novel chitosan grafted zinc containing nanoclay polymer biocomposite (CZNCPC): Controlled release formulation (CRF) of Zn²⁺. In *REACTIVE & FUNCTIONAL POLYMERS*. ISSN 1381-5148, JUN 2018, vol. 127, p. 55-66., Registrované v: WOS
4. [1.1] WU, J. - LI, K.C. - PAN, X.M. - LIAO, S.Q. - YOU, J.H. - ZHU, K.Z. - WANG, Z.F. Preparation and Physical Properties of Porous Starch/Natural Rubber Composites. In *STARCH-STARKE*. ISSN 0038-9056, NOV 2018, vol. 70, no. 11-12., Registrované v: WOS

ADCA142 HRACHOVÁ, Jana - MADEJOVÁ, Jana - BILLIK, Peter - KOMADEL, Peter - FAJNOR, Vladimír Štefan. Dry grinding of Ca and octadecyltrimethylammonium montmorillonite. In *Journal of Colloid and Interface Science*, 2007, vol. 316, no. 2, p. 589-595. (2007 - Current Contents). ISSN 0021-9797.

Citácie:

1. [1.1] CHICINAS, R. Plesa - BEDELEAN, H. - STEFAN, R. - MAICANEANU, A. Ability of a montmorillonitic clay to interact with cationic and anionic dyes in aqueous solutions. In *JOURNAL OF MOLECULAR STRUCTURE*. ISSN 0022-2860, 2018, vol. 1154, no., pp. 187-195., Registrované v: WOS

ADCA143 HRDÁ, Marcela - KULICH, Tomáš - REPISKÝ, Michal - NOGA, Jozef - MALKINA, Oľga - MALKIN, Vladimír. Implementation of the diagonalization-free algorithm in the self-consistent field procedure within the four-component relativistic scheme. In *Journal of Computational Chemistry*, 2014, vol. 35, no. 23, p. 1725-1737. (2013: 3.601 - IF, 1.449 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 0192-8651.

Citácie:

1. [1.1] UHLIKOVA, Tereza - URBAN, Stepan. *Ab initio NMR parameters of BrCH₃ and ICH₃ with relativistic and vibrational corrections. In MOLECULAR PHYSICS. ISSN 0026-8976, 2018, vol. 116, no. 9, pp. 1192-1197., Registrované v: WOS*
- ADCA144 HRICOVÍNI, Miloš - SCHOLTZOVÁ, Eva - BÍŽIK, F. B3LYP/6-311++G** study of structure and spin-spin coupling constant in heparin disaccharide. In *Carbohydrate Research*, 2007, vol. 342, no. 10, p. 1350-1356. (2006: 1.703 - IF, karentované - CCC). (2007 - Current Contents). ISSN 0008-6215.

Citácie:

1. [1.1] BESTAOUI-BERREKHCHI-BERRAHMA, N. - SPRINGBORG, M. - BERREKHCHI-BERRAHMA, C. A. - SEKKAL-RAHAL, M. *DFT and MP2 conformational study of 3,6-anhydro-alpha-D-galactose in gas phase and in aqueous solvent. In COMPUTATIONAL AND THEORETICAL CHEMISTRY. ISSN 2210-271X, 2018, vol. 1126, no., pp. 44-53., Registrované v: WOS*
- ADCA145 HRICOVÍNI, Miloš - DRIGUEZ, Pierre-Alexandre - MALKINA, Olga. NMR and DFT analysis of trisaccharide from heparin repeating sequence. In *Journal of Physical Chemistry B*, 2014, vol. 118, no. 41, p. 11931-11942. (2013: 3.377 - IF, 1.494 - SJR, karentované - CCC). (2014 - Current Contents, WOS, SCOPUS). ISSN 1520-6106.

Citácie:

1. [1.1] ALMOND, Andrew. *Multiscale modeling of glycosaminoglycan structure and dynamics: current methods and challenges. In CURRENT OPINION IN STRUCTURAL BIOLOGY. ISSN 0959-440X, 2018, vol. 50, no., pp. 58-64., Registrované v: WOS*
2. [1.1] FARRELL, Nicholas P. - GORLE, Anil K. - PETERSON, Erica J. - BERNERS-PRICE, Susan J. *Metalloglycomics. In METALLO-DRUGS: DEVELOPMENT AND ACTION OF ANTICANCER AGENTS. ISSN 1559-0836, 2018, vol. 18, no., pp. 109-140., Registrované v: WOS*
3. [1.1] MOHAMED, Slim Hadj - QUERTINMONT, Jean - DELBAERE, Stephanie - SANGUINET, Lionel - CHAMPAGNE, Benoit. *Assessing the Structure of Octastate Molecular Switches Using H-1 NMR Density Functional Theory Calculations. In JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, 2018, vol. 122, no. 3, pp. 1800-1808., Registrované v: WOS*
- ADCA146 HROBÁRIK, Peter - HROBÁRIKOVÁ, Veronika - MEIER, Florian - REPISKÝ, Michal - KOMOROVSKÝ, Stanislav - KAUPP, Martin. Relativistic four-component DFT calculations of ¹H NMR chemical shifts in transition-metal hydride complexes: unusual high-field shifts beyond the Buckingham-Stephens model. In *Journal of Physical Chemistry A*, 2011, vol. 115, no. 22, p. 5654-5659. (2010: 2.732 - IF, karentované - CCC). (2011 - Current Contents). ISSN 1089-5639.

Citácie:

1. [1.1] BERTRAND, Benoit - BOCHMANN, Manfred - FERNANDEZ-CESTAU, Julio - ROCCHIGIANI, Luca. *Pincer Complexes of Gold: An Overview of Synthesis, Reactivity, Photoluminescence, and Biological Applications. In PINCER COMPOUNDS: CHEMISTRY AND APPLICATIONS, 2018, vol., no., pp. 673-699., Registrované v: WOS*
2. [1.1] LEVESON-GOWER, Reuben B. - WEBB, Paul B. - CORDES, David B. - SLAWIN, Alexandra M. Z. - SMITH, David M. - TOOZE, Robert P. - LIU, Jianke. *Synthesis, Characterization, and Catalytic Properties of Iridium Pincer Complexes Containing NH Linkers. In ORGANOMETALLICS. ISSN 0276-7333, 2018, vol. 37, no. 1, pp. 30-39., Registrované v: WOS*
3. [1.1] OTT, Jonas C. - WADEPOHL, Hubert - ENDERS, Markus - GADE, Lutz H. *Taking Solution Proton NMR to Its Extreme: Prediction and Detection of a Hydride Resonance in an Intermediate-Spin Iron Complex. In JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. ISSN 0002-7863, 2018, vol. 140, no. 50, pp. 17413-17417., Registrované v: WOS*
4. [1.1] RUMPEL, Sigrun - SOMMER, Constanze - REIJERSE, Edward - FARES, Christophe - LUBITZ, Wolfgang. *Direct Detection of the Terminal Hydride Intermediate in [FeFe] Hydrogenase by NMR Spectroscopy. In JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. ISSN 0002-7863, 2018, vol. 140, no. 11, pp. 3863-3866., Registrované v: WOS*
5. [1.1] SZELL, Patrick M. J. - CAVALLO, Gabriella - TERRANEO, Giancarlo - METRANGOLO, Pierangelo - GABIDULLIN, Bulat - BRYCE, David L. *Comparing the Halogen Bond to the Hydrogen Bond by Solid-State NMR Spectroscopy: Anion Coordinated Dimers from 2-and 3-Iodoethynylpyridine Salts. In CHEMISTRY-A EUROPEAN JOURNAL. ISSN 0947-6539, 2018, vol. 24, no. 44, pp. 11364-11376., Registrované v: WOS*
- ADCA147 HROBÁRIK, Peter - REPISKÝ, Michal - KOMOROVSKÝ, Stanislav - HROBÁRIKOVÁ, Veronika - KAUPP, Martin. Assessment of higher-order spin-orbit effects on electronic g-tensors of d1 transition-metal complexes by relativistic two- and four-component methods. In *Theoretical Chemistry Accounts*, 2011, vol. 129, no 3-5, p. 715-725. (2010: 2.903 - IF, karentované - CCC). (2011 - Current Contents). ISSN 1432-881X.

Citácie:

1. [1.1] FERNANDEZ, Estefania - MORENO-GONZALEZ, Marta - MOLINER, Manuel - BLASCO, Teresa - BORONAT, Mercedes - CORMA, Avelino. *Modeling of EPR Parameters for Cu(II): Application to the Selective Reduction of NO_x Catalyzed by Cu-Zeolites. In TOPICS IN CATALYSIS. ISSN 1022-5528, 2018, vol. 61, no. 9-11, pp. 810-832., Registrované v: WOS*
2. [1.1] SINGH, Saurabh Kumar - ATANASOV, Mihail - NEESE, Frank. *Challenges in Multireference Perturbation Theory for the Calculations of the g-Tensor of First-Row Transition-Metal Complexes. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 9, pp. 4662-4677., Registrované v: WOS*
- ADCA148 HROBÁRIK, Peter - SIGMUNDOVÁ, Ivica - ZAHRADNÍK, Pavol - KASÁK, Peter - ARION, Vladimír - FRANZ, Edith - CLAYS, Koen. Molecular engineering of benzothiazolium salts with large quadratic hyperpolarizabilities: Can auxiliary electron-withdrawing groups enhance nonlinear optical responses? In *Journal of Physical Chemistry C*, 2010, vol. 114, no. 50, p. 22289-22302. (2009: 4.224 - IF, karentované - CCC). (2010 - Current Contents). ISSN 1932-7447.

Citácie:

1. [1.1] AZIZ, S.G. - OSMAN, O.I. - ELROBY, S.A. - HASSAN, W.M.I. - JEDIDI, A. - HILAL, R.H. *Proton-coupled electron transfer in dye-sensitized solar cells: a theoretical perspective. In STRUCTURAL CHEMISTRY. ISSN 1040-0400, AUG 2018, vol. 29, no. 4, p. 983-997., Registrované v: WOS*
2. [1.1] JAGADESAN, A. - SIVAKUMAR, N. - KUMAR, R.M. - CHAKKARAVARTHI, G. - ARJUNAN, S. *Synthesis, crystal*

- structure, growth and characterization of an optical organic material: 4-Aminopyridinium Trichloro acetate single crystal. In *OPTICAL MATERIALS*. ISSN 0925-3467, OCT 2018, vol. 84, p. 864-869., Registrované v: WOS
3. [1.1] KATLA, J. - HAZRA, B. - VERMA, M.S. - PALAKOLLU, V. - NAGARAJU, S. - CHANDRA, M. - KANVAH, S. Donor-Acceptor Styrylisoaxazoles: Solvatochromism and Large First Hyperpolarizability. In *CHEMISTRYSELECT*. ISSN 2365-6549, JUL 6 2018, vol. 3, no. 25, p. 7416-7421., Registrované v: WOS
4. [1.1] REN, T.B. - XU, W. - ZHANG, W. - ZHANG, X.X. - WANG, Z.Y. - XIANG, Z. - YUAN, L. - ZHANG, X.B. A General Method To Increase Stokes Shift by Introducing Alternating Vibronic Structures. In *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*. ISSN 0002-7863, JUN 20 2018, vol. 140, no. 24, p. 7716-7722., Registrované v: WOS
5. [1.1] SHIN, M.H. - LEE, S.H. - KANG, B.J. - JAZBINSEK, M. - YOON, W. - YUN, H. - ROTERMUND, F. - KWON, O.P. Organic Three-Component Single Crystals with Pseudo-Isomorphic Cocrystallization for Nonlinear Optics and THz Photonics. In *ADVANCED FUNCTIONAL MATERIALS*. ISSN 1616-301X, NOV 28 2018, vol. 28, no. 48., Registrované v: WOS
6. [1.1] SUNDARAM, S.J. - RAMACLUS, J.V. - ANTONY, P. - JACCOB, M. - SAGAYARAJ, P. Synthesis, growth and characterization of a new acentric 4-[4-(4-dimethylamino-phenyl)buta-1,3-dienyl]-1-methyl pyridinium p-chlorobenzenesulfonate dihydrate crystal for nonlinear optical applications. In *NEW JOURNAL OF CHEMISTRY*. ISSN 1144-0546, DEC 7 2018, vol. 42, no. 23, p. 18865-18872., Registrované v: WOS
7. [1.1] WEN, L.F. - FANG, Y. - YANG, J.Y. - HAN, Y.B. - SONG, Y.L. Third-order nonlinear optical properties and ultrafast excited-state dynamics of benzothiazolium salts: Transition in absorption and refraction under different time regimes. In *DYES AND PIGMENTS*. ISSN 0143-7208, SEP 2018, vol. 156, p. 26-32., Registrované v: WOS

ADCA149 HROBÁRIK, Peter - MALKINA, Oľga - MALKIN, Vladimír - KAUPP, Martin. Relativistic two-component calculations of electronic g-tensor for oxo-molybdenum(V) and oxo-tungsten(V) complexes: The important role of higher-order spin-orbit contributions. In *Chemical Physics*, 2009, vol. 356, no. 1-3, p. 229-235. (2008: 1.961 - IF, karentované - CCC). (2009 - Current Contents).

Citácie:

1. [1.1] WELLER, Tobias - DEILMANN, Leonie - TIMM, Jana - DOERR, Tobias S. - BEAUCAGE, Peter A. - CHEREVAN, Alexey S. - WIESNER, Ulrich B. - EDER, Dominik - MARSCHALL, Roland. A crystalline and 3D periodically ordered mesoporous quaternary semiconductor for photocatalytic hydrogen generation. In *NANOSCALE*. ISSN 2040-3364, 2018, vol. 10, no. 7, pp. 3225-3234., Registrované v: WOS

ADCA150 HROBÁRIK, Peter - HORVÁTH, Branislav - SIGMUNDOVÁ, Ivica - ZAHRADNÍK, Pavol - MALKINA, Oľga. The impact of the pi-electron conjugation on ¹⁵N, ¹³C and ¹H NMR chemical shifts in push-pull benzothiazolium salts. Experimental and theoretical study. In *Magnetic Resonance in Chemistry*, 2007, vol. 45, no. 11, p. 942-953. (2006: 1.610 - IF, karentované - CCC). (2007 - Current Contents).

Citácie:

1. [1.1] CHEN, Yue - LI, Duxin - YANG, Wenyan - XIAO, Chunguang - WEI, Mengling. Effects of different amine-functionalized graphene on the mechanical, thermal, and tribological properties of polyimide nanocomposites synthesized by in situ polymerization. In *POLYMER*. ISSN 0032-3861, 2018, vol. 140, no., pp. 56-72., Registrované v: WOS

ADCA151 HROBÁRIK, Peter - REVIKINE, Roman - ARBUZNIKOV, Alexei V. - MALKINA, Oľga - MALKIN, Vladimír - KÖHLER, Frank H. - KAUPP, Martin. Density functional calculations of NMR shielding tensors for paramagnetic systems with arbitrary spin multiplicity: Validation on 3d metallocenes. In *Journal of Chemical Physics*, 2007, vol. 126, no. 2, p. 024107-1-024107-19. (2007 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] JEREMIAS, Lukas - NOVOTNY, Jan - REPISKY, Michal - KOMOROVSKY, Stanislav - MAREK, Radek. Interplay of Through-Bond Hyperfine and Substituent Effects on the NMR Chemical Shifts in Ru(III) Complexes. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 15, p. 8748-8759., Registrované v: WOS
2. [1.1] MARES, Jiri - VAARA, Juha. Ab initio paramagnetic NMR shifts via point-dipole approximation in a large magnetic-anisotropy Co(II) complex. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 35, pp. 22547-22555., Registrované v: WOS
3. [1.1] NOVOTNY, Jan - PRICHYSTAL, David - SOJKA, Martin - KOMOROVSKY, Stanislav - NECAS, Marek - MAREK, Radek. Hyperfine Effects in Ligand NMR: Paramagnetic Ru(III) Complexes with 3-Substituted Pyridines. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 2, pp. 641-652., Registrované v: WOS
4. [1.1] SERGENTU, Dumitru-Claudiu - GENDRON, Frederic - AUTSCHBACH, Jochen. Similar ligand-metal bonding for transition metals and actinides? 5f(1) U(C7H7)(2)(-) versus 3d(n) metallocenes. In *CHEMICAL SCIENCE*. ISSN 2041-6520, 2018, vol. 9, no. 29, pp. 6292-6306., Registrované v: WOS

ADCA152 HUANG, Yu Li - WRUSS, Elisabeth - EGGER, David A. - KERA, Satoshi - UENO, Nobuo - SAIDI, Wissam A. - BUČKO, Tomáš - WEE, Andrew T.S. - ZOJER, Egbert. Understanding the adsorption of CuPc and ZnPc on noble metal surfaces by combining quantum-mechanical modelling and photoelectron spectroscopy. In *Molecules*, 2014, vol. 19, no. 3, p. 2969-2992. (2013: 2.095 - IF, 0.707 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 1420-3049.

Citácie:

1. [1.1] BIRMINGHAM, Blake - LIEGE, Zachary - LARSON, Nick - LU, Weigang - PARK, Kenneth T. - LEE, Ho Wai Howard - VORONINE, Dmitri V. - SCULLY, Marlan O. - ZHANG, Zhenrong. Probing Interaction between Individual Submonolayer Nanoislands and Bulk MoS₂ Using Ambient TERS. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 5, pp. 2753-2760., Registrované v: WOS
2. [1.1] BUIMAGA-LARINCA, L. - MORARI, C. Translation of metal-phthalocyanines adsorbed on Au(111): from van der Waals interaction to strong electronic correlation. In *SCIENTIFIC REPORTS*. ISSN 2045-2322, 2018, vol. 8, no., pp., Registrované v: WOS

3. [1.1] DREHER, Maximilian - BISCHOF, Daniel - WIDDASCHECK, Felix - HUTTNER, Andrea - BREUER, Tobias - WITTE, Gregor. *Interface Structure and Evolution of Dinaphthothienothiophene (DNNT) Films on Noble Metal Substrates*. In *ADVANCED MATERIALS INTERFACES*. ISSN 2196-7350, 2018, vol. 5, no. 21, pp., Registrované v: WOS
 4. [1.1] VAN STRAATEN, Gerben - FRANKE, Markus - SOUBATCH, Serguei - STADTMUELLER, Benjamin - DUNCAN, David A. - LEE, Tien-Lin - TAUTZ, F. Stefan - KUMPF, Christian. *Role of the Central Metal Atom in Substrate-Mediated Molecular Interactions in Phthalocyanine-Based Heteromolecular Monolayers*. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 15, pp. 8491-8504., Registrované v: WOS
- ADCA153 CHERRY, Peter - MALKIN, Vladimír - MALKINA, Oľga - ASHER, James Richard. Energy anisotropy as a function of the direction of spin magnetization for a doublet system. In *Journal of Chemical Physics*, 2016, vol. 145, no. 17, p. 174108-1-174108-5. (2015: 2.894 - IF, Q2 - JCR, 0.953 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0021-9606.
- Citácie:
1. [1.1] WODYNSKI, Artur - KAUPP, Martin. *Noncollinear Two-Component Quasirelativistic Description of Spin Interactions in Exchange-Coupled Systems. Mapping Generalized Broken-Symmetry States to Effective Spin Hamiltonians*. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 3, pp. 1267-1276., Registrované v: WOS
- ADCA154 CHERRY, Peter - KOMOROVSKÝ, Stanislav - MALKIN, Vladimír - MALKINA, Oľga. Calculations of the EPR g-tensor using unrestricted two- and four-component relativistic approaches within the HF and DFT frameworks. In *Molecular Physics*, 2017, vol. 115, no. 1-2, p. 75-89. (2016: 1.870 - IF, Q2 - JCR, 0.820 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0026-8976.
- Citácie:
1. [1.1] SINGH, Saurabh Kumar - ATANASOV, Mihail - NEESE, Frank. *Challenges in Multireference Perturbation Theory for the Calculations of the g-Tensor of First-Row Transition-Metal Complexes*. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 9, pp. 4662-4677., Registrované v: WOS
- ADCA155 CHIBANI, Siwar - CHEBBI, Mouheb - LEBÈGUE, Sébastien - BUČKO, Tomáš - BADAWI, Michael. A DFT investigation of the adsorption of iodine compounds and water in H-, Na-, Ag-, and Cu-mordenite. In *Journal of Chemical Physics*, 2016, vol. 144, no. 24, p. 244705-1-244705-10. (2015: 2.894 - IF, Q2 - JCR, 0.953 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0021-9606.
- Citácie:
1. [1.1] CANTREL, Laurent - ALBIOL, Thierry - BOSLAND, Loic - COLOMBANI, Juliette - COUSIN, Frederic - GREGOIRE, Anne-Cecile - LEROY, Olivia - MORIN, Sandrine. *Research Works on Iodine and Ruthenium Behavior in Severe Accident Conditions*. In *JOURNAL OF NUCLEAR ENGINEERING AND RADIATION SCIENCE*. ISSN 2332-8983, 2018, vol. 4, no. 2, pp., Registrované v: WOS
 2. [1.1] CHUN, Hoje - KANG, Joonhee - HAN, Byungchan. *Universal Scaling Relationship To Screen an Efficient Metallic Adsorbent for Adsorptive Removal of Iodine Gas under Humid Conditions: First-Principles Study*. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 22, pp. 11799-11806., Registrované v: WOS
 3. [1.1] HUVE, Joffrey - RYZHIKOV, Andrey - NOUALI, Habiba - LALIA, Virginie - AUGÉ, Gregoire - DAOU, T. Jean. *Porous sorbents for the capture of radioactive iodine compounds: a review*. In *RSC ADVANCES*. ISSN 2046-2069, 2018, vol. 8, no. 51, pp. 29248-29273., Registrované v: WOS
 4. [1.1] NAN, Yue - LIU, Jiuxu - TANG, Siqi - LIN, Ronghong - TAVLARIDES, Lawrence L. *Silver-Exchanged Mordenite for Capture of Water Vapor in Off-Gas Streams: A Study of Adsorption Kinetics*. In *INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH*. ISSN 0888-5885, 2018, vol. 57, no. 3, pp. 1048-1058., Registrované v: WOS
- ADCA156 CHOVANEC, Jozef - CHROMČÍKOVÁ, Mária - LIŠKA, Marek - SHÁNĚLOVÁ, J. - MÁLEK, J. Thermodynamic model and viscosity of Ge-S glasses. In *Journal of Thermal Analysis and Calorimetry*, 2014, vol. 116, no. 2, p. 581-588. (2013: 2.206 - IF, 0.458 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 1388-6150. (Vega 1/0006/12 : Štruktúra a vlastnosti oxidových skiel - molekulová dynamika, termodynamické modely, kryštalizácia, vibračné a impedančné spektrá. ITMS 26220220084 : Znalostná databáza a expertný systém environmentálneho riešenia havárií straty chladiva v prevádzke jadrovej elektrárne).
- Citácie:
1. [1.1] CHAHAL, R. - STARECKI, F. - DOUALAN, J-L - NEMEC, P. - TRAPANANTI, A. - PRESTIPIN, C. - TRICOT, G. - BOUSSARD-PLEDEL, C. - MICHEL, K. - BRAUD, A. - CAMY, P. - ADAM, J-L - BUREAU, B. - NAZABAL, And. *Nd³⁺: Ga-Ge-Sb-S glasses and fibers for luminescence in mid-IR: synthesis, structural characterization and rare earth spectroscopy*. In *OPTICAL MATERIALS EXPRESS*. ISSN 2159-3930, 2018, vol. 8, no. 6, pp. 1650-1671., Registrované v: WOS
 2. [1.1] KOZMIDIS-PETROVIC, Ana - SESTAK, Jaroslav. *Glass transition temperature its exploitation and new conception of fragility*. In *PHYSICS AND CHEMISTRY OF GLASSES-EUROPEAN JOURNAL OF GLASS SCIENCE AND TECHNOLOGY PART B*. ISSN 1753-3562, 2018, vol. 59, no. 6, pp. 259-266., Registrované v: WOS
 3. [1.1] ZHAO, Xuhao - YU, Mingqiang - YU, Xinlan - LIN, Changgui. *Physical and structural properties of Ge-rich chalcogenide glass sandwiched by GeS crystalline layers*. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 12, pp. 13827-13831., Registrované v: WOS
- ADCA157 CHOVANEC, Jozef - SVOBODA, Roman - KRAXNER, Jozef - ČERNÁ, Andrea - GALUSEK, Dušan. Crystallization kinetics of the Y3Al5O12 glass. In *Journal of Alloys and Compounds*, 2017, vol. 725, p. 792-799. (2016: 3.133 - IF, Q1 - JCR, 0.954 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0925-8388.
- Citácie:
1. [1.1] MA, Xiaoguang - LI, Xiaoyu - LI, Jianqiang - GENEVOIS, Cecile - MA, Bingqian - ETIENNE, Auriane - WAN, Chunlei - VERON, Emmanuel - PENG, Zhijian - ALLIX, Mathieu. *Pressureless glass crystallization of transparent yttrium aluminum garnet-*

based nanoceramics. In *NATURE COMMUNICATIONS*. ISSN 2041-1723, 2018, vol. 9, no., pp., Registrované v: WOS

2. [1.1] MRAZEK, Jan - KASIK, Ivan - PROCHAZKOVA, Lenka - CUBA, Vaclav - GIRMAN, Vladimir - PUCHY, Viktor - BLANC, Wilfried - PETERKA, Pavel - AUBRECHT, Jan - CAJZL, Jakub - PODRAZKY, Ondrej. YAG Ceramic Nanocrystals Implementation into MCVD Technology of Active Optical Fibers. In *APPLIED SCIENCES-BASEL*. ISSN 2076-3417, 2018, vol. 8, no. 5, pp., Registrované v: WOS

ADCA158 CHOVANEC, Jozef - GALUSEK, Dušan - RÁHEL, Jozef - ŠAJGALÍK, Pavol. Low loss alumina dielectrics by aqueous tape casting: The influence of composition on the loss tangent. In *Ceramics International*, 2012, vol. 38, no. 5, p. 3747-3755. (2011: 1.751 - IF, 0.922 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] TOHIDIFAR, Mohammad Reza. Highly-efficient electromagnetic interference shielding and microwave dielectric behavior of a (Bi₂O₃ + B₂O₃)-doped MWCNT/BaTiO₃ ceramic nanocomposite. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 12, pp. 13613-13622., Registrované v: WOS

ADCA159 CHRAPPOVÁ, Jana - SCHWENDT, Peter - SIVÁK, Michal - REPISKÝ, Michal - MALKIN, Vladimír - MAREK, Jaromír. Dinuclear fluoro-peroxovanadium(V) complexes with symmetric and asymmetric peroxo bridges: syntheses, structures and DFT studies. In *Dalton Transactions*, 2009, no. 3, p. 465-473. (2008: 3.580 - IF). ISSN 1477-9226.

Citácie:

1. [1.1] CHAHKANDI, Mohammad - ALIABAD, H. A. Rahnamaye. Role of hydrogen bonding in establishment of a crystalline network of Cu (II) complex with hydrazone-derived ligand: optoelectronic studies. In *CHEMICAL PAPERS*. ISSN 2585-7290, 2018, vol. 72, no. 5, pp. 1287-1297., Registrované v: WOS

2. [1.1] RAHMATI, Zahra - MIRZAEI, Masoud - CHAHKANDI, Mohammad - MAGUE, Joel T. Accurate DFT studies on crystalline network formation of a new Co(II) complex bearing 8-aminoquinoline. In *INORGANICA CHIMICA ACTA*. ISSN 0020-1693, 2018, vol. 473, no., pp. 152-159., Registrované v: WOS

3. [1.1] XIE, Tian-xin - CHU, Fu-hao - YAN, Wen-qiang - XU, Bing - CHEN, Jing - ZHAO, Rui - ZHANG, Yu-zhong - WANG, Peng-long - LEI, Hai-min. Synthesis and biological evaluation of new peroxo-bridged diosgenin derivatives. In *CHINESE HERBAL MEDICINES*. ISSN 1674-6384, 2018, vol. 10, no. 1, pp. 54-58., Registrované v: WOS

ADCA160 CHRENKOVÁ, Marta - SILNÝ, A. - ŠIMKO, František - THONSTAD, J. Density of the NaAlF₄ + KAlF₄ electrolyte, saturated with alumina. In *Journal of Chemical and Engineering Data*, 2010, vol. 55, p. 3438-3440. (2009: 1.695 - IF).

Citácie:

1. [1.1] KUBIKOVA, Blanka - MLYNARIKOVA, Jarmila - BOCA, Miroslav - SHI, Zhongning - GAO, Bingliang - PATEL, Niketan. Temperatures of Primary Crystallization and Density of the KF + AlF₃ + LiF + Al₂O₃ Molten System. In *JOURNAL OF CHEMICAL AND ENGINEERING DATA*. ISSN 0021-9568, 2018, vol. 63, no. 8, pp. 3047-3052., Registrované v: WOS

ADCA161 CHROMČÍKOVÁ, Mária - LIŠKA, Marek - LISSOVÁ, Magdaléna - MOŠNER, Petr - KOUDELKA, Ladislav. Structural relaxation of PbO-WO₃-P₂O₅ glasses. In *Journal of Thermal Analysis and Calorimetry*, 2013, vol. 114, no. 3, p. 947-954. (2012: 1.982 - IF, 0.596 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 1388-6150. (Vega 1/0006/12 : Štruktúra a vlastnosti oxidových skiel - molekulová dynamika, termodynamické modely, kryštalizácia, vibračné a impedančné spektrá. ITMS 26220220084 : Znalostná databáza a expertný systém environmentálneho riešenia havárií straty chladiva v prevádzke jadrovej elektrárne. APVV-0487-11 : Štruktúra a vlastnosti oxidových skiel určených na aplikácie v jadrovej energetike).

Citácie:

1. [1.1] KOZMIDIS-PETROVIC, Ana - SESTAK, Jaroslav. Glass transition temperature its exploitation and new conception of fragility. In *PHYSICS AND CHEMISTRY OF GLASSES-EUROPEAN JOURNAL OF GLASS SCIENCE AND TECHNOLOGY PART B*. ISSN 1753-3562, 2018, vol. 59, no. 6, pp. 259-266., Registrované v: WOS

ADCA162 CHROMČÍKOVÁ, Mária - DEJ, P. Structural relaxation of NBS711 glass - Reliability of the regression estimates of relaxation model. In *Ceramics-Silikáty*, 2006, vol. 50, no. 3, p. 125-129. (2005: 0.463 - IF, karentované - CCC). (2006 - Current Contents). ISSN 0862-5468.

Citácie:

1. [1.1] KOSTAL, Petr - HOFIREK, Tomas - MALEK, Jiri. Viscosity measurement by thermomechanical analyzer. In *JOURNAL OF NON-CRYSTALLINE SOLIDS*. ISSN 0022-3093, 2018, vol. 480, no., pp. 118-122., Registrované v: WOS

ADCA163 IBRAHIM, Ismail - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol - BENCO, Ľubomír. Electronic structure and energy level schemes of RE₃+:LaSi₃N₅ and RE₂+:LaSi₃N₅-xO_x phosphors (RE=Ce, Pr, Nd, Pm, Sm, Eu) from first principles. In *Journal of Luminescence*, 2015, vol. 164, p. 131-137. (2014: 2.719 - IF, Q1 - JCR, 0.811 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0022-2313.

Citácie:

1. [1.1] ZHANG, Yongyang - DING, Bangfu - YIN, Luqiao - XIN, Jiandi - ZHAO, Rui - ZHENG, Shukai - YAN, Xiaobing. Monoclinic Lu₂-xSm_xWO₆-Based White Light-Emitting Phosphors: From Ground-Excited-States Calculation Prediction to Experiment Realization. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 1, pp. 507-518., Registrované v: WOS

ADCA164 IBRAHIM, Ismail - LENČEŠ, Zoltán - BENCO, Ľubomír - HRABALOVÁ, Monika - ŠAJGALÍK, Pavol. Cerium-doped LaSi₃N₅: Computed electronic structure and band gaps. In *Journal of the European Ceramic Society*, 2014, vol. 34, no. 11, p. 2705-2712. (2013: 2.307 - IF, 1.122 - SJR, karentované - CCC). (2014 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] EHRE, F. - LABBE, C. - DUFOUR, C. - JADWISIENCZAK, W. M. - WEIMMERSKIRCH-AUBATIN, J. - PORTIER, X. -

DOUALAN, J-L - CARDIN, J. - RICHARD, A. L. - INGRAM, D. C. - LABRUGERE, C. - GOURBILLEAU, F. The nitrogen concentration effect on Ce doped SiO_xNy emission: towards optimized Ce³⁺ for LED applications. In NANOSCALE. ISSN 2040-3364, 2018, vol. 10, no. 8, pp. 3823-3837., Registrované v: WOS

2. [1.1] WANG, Shuxin - SONG, Zhen - KONG, Yuwei - XIA, Zhiguo - LIU, Quanlin. Crystal field splitting of 4f(n-1)5d-levels of Ce³⁺ and Eu²⁺ in nitride compounds. In JOURNAL OF LUMINESCENCE. ISSN 0022-2313, 2018, vol. 194, no., pp. 461-466., Registrované v: WOS

ADCA165 IBRAHIM, Ismail - LENČEŠ, Zoltán - BENCO, Ľubomír - ŠAJGALÍK, Pavol. Lanthanide-doped LaSi₃N₅ based phosphors: Ab initio study of electronic structures, band gaps, and energy level locations. In Journal of Luminescence, 2016, vol. 172, p. 83-91. (2015: 2.693 - IF, Q1 - JCR, 0.787 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0022-2313.

Citácie:

1. [1.1] ZHANG, Yongyang - DING, Bangfu - YIN, Luqiao - XIN, Jiandi - ZHAO, Rui - ZHENG, Shukai - YAN, Xiaobing. Monoclinic Lu_{2-x}Sm_xWO₆-Based White Light-Emitting Phosphors: From Ground-Excited-States Calculation Prediction to Experiment Realization. In INORGANIC CHEMISTRY. ISSN 0020-1669, 2018, vol. 57, no. 1, pp. 507-518., Registrované v: WOS

2. [1.1] ZHANG, Yongyang - XIN, Jiandi - ZHENG, Huibing - ZHAO, Zhengui - ZHANG, Junying - YANG, Yanmin - ZHENG, Shukai - ZHAO, Rui - DING, Bangfu. Yb³⁺ Doping Monoclinic Lu₂WO₆: Near-Infrared Emission and Energy-Transfer Luminescence Mechanism. In JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, 2018, vol. 122, no. 37, pp. 21607-21616., Registrované v: WOS

ADCA166 IBRAHIM, Ismail - LENČEŠ, Zoltán - BENCO, Ľubomír - HRABALOVÁ, Monika - ŠAJGALÍK, Pavol. Sm-doped LaSi₃N₅: Synthesis, computed electronic structure, and band gaps. In Journal of the American Ceramic Society, 2014, vol. 97, no. 8, p. 2546-2551. (2013: 2.428 - IF, 1.168 - SJR, karentované - CCC). (2014 - Current Contents, WOS, SCOPUS). ISSN 0002-7820.

Citácie:

1. [1.1] CHEN HAITAO - HUANG XUEFEI - HUANG WEIGANG. Effect of manganese on the crystal structures and luminescence properties of mn doped Sr₂SiO₄:Eu²⁺ phosphors. In CHINESE JOURNAL OF PHYSICS. ISSN 0577-9073, 2018, vol. 56, no. 5, pp. 1977-1984., Registrované v: WOS

2. [1.1] ZHANG, Xian - LI, Zhao - ZENG, Qingfeng. First-principles calculation on the electronic structure and optical properties of Eu²⁺ doped gamma-AlON phosphor. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 2, pp. 1461-1466., Registrované v: WOS

ADCA167 JANKOVIČ, Ľuboš - MADEJOVÁ, Jana - KOMADEL, Peter - JOCHEC MOŠKOVÁ, Daniela - CHODÁK, Ivan. Characterization of systematically selected organo-montmorillonites for polymer nanocomposites. In Applied Clay Science, 2011, vol. 51, p. 438 - 444. (2010: 2.303 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] SONI, V.K. - ROY, T. - DHARA, S. - CHOUDHARY, G. - SHARMA, P.R. - SHARMA, R.K. On the investigation of acid and surfactant modification of natural clay for photocatalytic water remediation. In JOURNAL OF MATERIALS SCIENCE. ISSN 0022-2461, JUL 2018, vol. 53, no. 14, p. 10095-10110., Registrované v: WOS

2. [1.1] TOMIC, M. - DUNJIC, B. - NIKOLIC, M.S. - MALETASKIC, J. - PAVLOVIC, V.B. - BAJAT, J. - DJONLAGIC, J. Dispersion efficiency of montmorillonites in epoxy nanocomposites using solution intercalation and direct mixing methods. In APPLIED CLAY SCIENCE. ISSN 0169-1317, MAR 15 2018, vol. 154, p. 52-63., Registrované v: WOS

ADCA168 JANKOVIČ, Ľuboš - KOMADEL, Peter. Metal cation-exchanged montmorillonite catalyzed protection of aromatic aldehydes with Ac₂O. In Journal of Catalysis, 2003, vol. 218, no. 1, p. 227-233. ISSN 0021-9517.

Citácie:

1. [1.1] LIU, Jie - WANG, Xue-Qian - YANG, Bei-Bei - LIU, Chun-Ling - XU, Chun-Li - DONG, Wen-Sheng. Highly efficient conversion of glucose into methyl levulinate catalyzed by tin-exchanged montmorillonite. In RENEWABLE ENERGY. ISSN 0960-1481, 2018, vol. 120, no., pp. 231-240., Registrované v: WOS

2. [1.1] WAHYUNI, Nelly - ZISSIS, Georges - MOULOUNGUI, Zephirin. Characterization of Acid Sites on Modified Kaolinite by FTIR Spectra of Pyridine Adsorbed. In 2ND INTERNATIONAL CONFERENCE ON CHEMISTRY, CHEMICAL PROCESS AND ENGINEERING (IC3PE). ISSN 0094-243X, 2018, vol. 2026, no., pp., Registrované v: WOS

ADCA169 JANOTKA, Ivan - MADEJOVÁ, Jana - ŠTEVULA, Ladislav - FRŤALOVÁ, D.M. Behaviour of Ca(OH)₂ in the presence of the set styrene-acrylate dispersion. In Cement and Concrete Research, 1996, vol. 26, no. 11, p. 1727-1735.

Citácie:

1. [1.1] LIU, Sifeng - KONG, Yaning - WAN, Tingting - ZHAO, Guorong. Effects of thermal-cooling cycling curing on the mechanical properties of EVA-modified concrete. In CONSTRUCTION AND BUILDING MATERIALS. ISSN 0950-0618, 2018, vol. 165, no., pp. 443-450., Registrované v: WOS

ADCA170 JÓNA, Eugen - LAJDOVÁ, Ľ. - LODUHOVÁ, M. - LENDVAYOVÁ, S. - PAVLÍK, Viliam - MONCOLE, J. - LIZÁK, P. - MOJUMDAR, Subhash Chandra. Thermal properties of solid complexes with biologically important heterocyclic ligands : Part IV. Thermal and spectral properties of 2-chloro- and 2-bromobenzoato Cu(II) complexes with nicotinamide and different bonded water molecules. In Journal of Thermal Analysis and Calorimetry, 2012, vol. 108, no. 3, p. 921-926. (2011: 1.604 - IF, 0.529 - SJR). ISSN 1388-6150.

Citácie:

1. [1.1] MARINESCU, Maria - POTMISCHIL, Francisc - FLOREA, Mihaela - CONSTANTINESCU, Catalin. Thermal behaviour of sym-octahydroacridines and their corresponding N(10)-oxides. In JOURNAL OF THERMAL ANALYSIS AND CALORIMETRY. ISSN 1388-6150, 2018, vol. 131, no. 1, pp. 117-125., Registrované v: WOS

- ADCA171 JÓNA, Eugen - RUDINSKÁ, G. - SAPIETOVÁ, M. - PAVLÍK, Viliam - DRÁBIK, Milan - MOJUMDAR, Subhash Chandra. Interactions of different heterocyclic compounds with monoionic forms of montmorillonite. Thermal, IR-spectral and X-ray studies of Ni(II)-montmorillonite with 3-R and 2-R pyridines (R=CH₃, Cl, NH₂). In *Journal of Thermal Analysis and Calorimetry*, 2007, vol. 90, no. 3, p. 687-691. (2006: 1.438 - IF, karentované - CCC). (2007 - Current Contents). ISSN 1388-6150.
Citácie:
1. [1.1] XU, Lin - LIU, Wei - CAI, Yawen - WU, Chunfang - CHEN, Lei - YANG, Shitong - WANG, Xiangke - JI, Guoxun - WANG, Shuao. Competitive sequestration of Ni(II) and Eu(III) on montmorillonite: role of molar Ni:Eu ratios and coexisting oxalate. In *ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH*. ISSN 0944-1344, 2018, vol. 25, no. 32, pp. 32617-32630., Registrované v: WOS
- ADCA172 KAHN, Kalju - KIRTMAN, Bernard - NOGA, Jozef - TEN-NO, Seiichiro. Anharmonic vibrational analysis of water with traditional and explicitly correlated coupled cluster methods. In *Journal of Chemical Physics*, 2010, vol. 133, no. 7, p. 074106-1-074106-12. (2009: 3.093 - IF, karentované - CCC). (2010 - Current Contents). ISSN 0021-9606.
Citácie:
1. [1.1] MORGAN, W. James - MATTHEWS, Devin A. - RINGHOLM, Magnus - AGARWAL, Jay - GONG, Justin Z. - RUUD, Kenneth - ALLEN, Wesley D. - STANTON, John F. - SCHAEFER, Henry F. Geometric Energy Derivatives at the Complete Basis Set Limit: Application to the Equilibrium Structure and Molecular Force Field of Formaldehyde. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 3, pp. 1333-1350., Registrované v: WOS
- ADCA173 KAHN, Kalju - GRANOVSKY, Alex A. - NOGA, Jozef. Convergence of third order correlation energy in atoms and molecules. In *Journal of Computational Chemistry*, 2007, vol. 28, no. 2, p. 547-554. ISSN 0192-8651.
Citácie:
1. [1.1] KARTON, Amir. Post-CCSD(T) contributions to total atomization energies in multireference systems. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 3, pp., Registrované v: WOS
- ADCA174 KARELL, Radovan - KRAXNER, Jozef - CHROMČÍKOVÁ, Mária - LIŠKA, Marek. Properties of selected zirconia containing silicate glasses II. In *Ceramics-Silikáty*, 2007, vol. 51, no. 3, p. 125-130. (2006: 0.597 - IF, karentované - CCC). (2007 - Current Contents). ISSN 0862-5468.
Citácie:
1. [1.1] LU, Xiaonan - DENG, Lu - DU, Jincheng. Effect of ZrO₂ on the structure and properties of soda-lime silicate glasses from molecular dynamics simulations. In *JOURNAL OF NON-CRYSTALLINE SOLIDS*. ISSN 0022-3093, 2018, vol. 491, no., pp. 141-150., Registrované v: WOS
2. [1.1] SOARES, Viviane O. - DAGUANO, Juliana K. M. B. - LOMBELLO, Christiane B. - BIANCHIN, Olavo S. - GONCALVES, Livia M. G. - ZANOTTO, Edgar D. New sintered wollastonite glass-ceramic for biomedical applications. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 16, pp. 20019-20027., Registrované v: WOS
- ADCA175 KARELL, Radovan - KRAXNER, Jozef - CHROMČÍKOVÁ, Mária. Properties of selected zirconia containing silicate glasses. In *Ceramics-Silikáty*, 2006, vol. 50, no. 2, p. 78-82. (2005: 0.463 - IF, karentované - CCC). (2006 - Current Contents). ISSN 0862-5468.
Citácie:
1. [1.1] GUO, Jicheng - VILLALON, Thomas - PAL, Uday - BASU, Soumendra. Effect of optical basicity on the stability of yttria-stabilized zirconia in contact with molten oxy-fluoride flux. In *JOURNAL OF THE AMERICAN CERAMIC SOCIETY*. ISSN 0002-7820, 2018, vol. 101, no. 8, pp. 3605-3616., Registrované v: WOS
2. [1.1] LU, Xiaonan - DENG, Lu - DU, Jincheng. Effect of ZrO₂ on the structure and properties of soda-lime silicate glasses from molecular dynamics simulations. In *JOURNAL OF NON-CRYSTALLINE SOLIDS*. ISSN 0022-3093, 2018, vol. 491, no., pp. 141-150., Registrované v: WOS
- ADCA176 KAŠIAROVÁ, Monika - TATARKO, Peter - BURIK, Peter - DUSZA, Ján - ŠAJGALÍK, Pavol. Thermal shock resistance of Si₃N₄ and Si₃N₄-SiC ceramics with rare-earth oxide sintering additives. In *Journal of the European Ceramic Society*, 2014, vol. 34, no. 14, p. 3301-3308. (2013: 2.307 - IF, 1.122 - SJR, karentované - CCC). (2014 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.
Citácie:
1. [1.1] FAN, Xingyu - WANG, Hongjie - NIU, Min - ZHANG, Dahai - ZHOU, Jun - FAN, Jinpeng. Experiments and transient finite element simulation of gamma-Y₂Si₂O₇/B₂O₃Al₂O₃-SiO₂ glass coating on porous Si₃N₄ substrate under thermal shock. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 4, pp. 4072-4079., Registrované v: WOS
2. [1.1] JIA, Dechang - LIANG, Bin - YANG, Zhihua - ZHOU, Yu. Metastable Si-B-C-N ceramics and their matrix composites developed by inorganic route based on mechanical alloying: Fabrication, microstructures, properties and their relevant basic scientific issues. In *PROGRESS IN MATERIALS SCIENCE*. ISSN 0079-6425, 2018, vol. 98, no., pp. 1-67., Registrované v: WOS
3. [1.1] SUN, Yangshan - CAI, Delong - YANG, Zhihua - LI, Qian - LI, Hailiang - JIA, Dechang - ZHOU, Yu. Thermal shock resistance of the porous boron nitride/silicon oxynitride ceramic composites. In *INTERNATIONAL JOURNAL OF APPLIED CERAMIC TECHNOLOGY*. ISSN 1546-542X, 2018, vol. 15, no. 6, pp. 1358-1365., Registrované v: WOS
4. [1.1] ZUO, Fei - MENG, Fan - LIN, Dong-Tao - LV, Jian - YU, Jun-Jie - CHEN, Qiang - WANG, Hong-Jian - HE, Fu-Po - SENGGER, Marco - LIN, Hua-Tay. Effect of current pattern and conductive phase on sintering behavior of Si₃N₄-based ceramic composite. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 8, pp. 9561-9567., Registrované v: WOS
- ADCA177 KAŠIAROVÁ, Monika - RUDNAYOVÁ, Emöke - DUSZA, Ján - HNATKO, Miroslav - ŠAJGALÍK, Pavol - MERSTALLINGER, A. - KUZSELLA, L. Some tribological properties of a carbon-derived Si₃N₄/SiC nanocomposite. In *Journal of the European Ceramic Society*, 2004, vol. 24, no. 12, p. 3431-3435. ISSN 0955-2219.

Citácie:

1. [1.1] SHARMA, Nidhi - ALAM, Syed Nasimul. Influence of Surface Roughness on Wear Behaviour of Ceramic Nanocomposites. In MATERIALS TODAY-PROCEEDINGS. ISSN 2214-7853, 2018, vol. 5, no. 14, pp. 28051-28060., Registrované v: WOS
- ADCA178 KAUPP, Martin - AUBAUER, Christoph - ENGELHARDT, Günter - KLAPÖTKE, Thomas M. - MALKINA, Oľga. The PI_4^+ cation has an extremely large negative $31P$ nuclear magnetic resonance chemical shift, due to spin-orbit coupling: A quantum-chemical prediction and its confirmation by solid-state nuclear magnetic resonance spectroscopy. In Journal of Chemical Physics, 1999, vol. 110, no. 8, p. 3897-3902. ISSN 0021-9606.

Citácie:

1. [1.1] ANGELES ALVAREZ, M. - CASADO-RUANO, Melodie - ESTHER GARCIA, M. - GARCIA-VIVO, Daniel - RUIZ, Miguel A. Dehydrogenation, Methyl Elimination and Insertion Reactionsofthe Agostic Methyl-Bridged Complex $[Mo_2Cp_2(\mu-kappa(1):eta(2)-CH_3)(\mu-PtBu_2)(\mu-CO)]$. In CHEMISTRY-A EUROPEAN JOURNAL. ISSN 0947-6539, 2018, vol. 24, no. 38, pp. 9504-9507., Registrované v: WOS
- ADCA179 KAUPP, Martin - GRESS, T. - REVIKINE, Roman - MALKIN, Vladimír - MALKINA, Oľga. g-tensor and spin density of the modified tyrosyl radical in galactose oxidase: A density functional study. In Journal of Physical Chemistry B, 2003, vol. 107, no. 1, p. 331-337. ISSN 1520-6106.

Citácie:

1. [1.1] GLASBRENNER, Michael - VOGLER, Sigurd - OCHSENFELD, Christian. Gauge-origin dependence in electronic g-tensor calculations. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 21, pp., Registrované v: WOS
- ADCA180 KAUPP, Martin - MALKIN, Vladimír - MALKINA, Oľga. The role of pi-type nonbonding orbitals for spin-orbit induced NMR chemical shifts: A DFT study of ^{13}C and ^{19}F shifts in the series CF_3IF_n ($n=0,2,4,6$). In Journal of Computational Chemistry, 1999, vol. 20, no. 12, p. 1304-1313. (1998: 2.860 - IF, karentované - CCC). (1999 - Current Contents). ISSN 0192-8651.

Citácie:

1. [1.1] RUSAKOV, Yu. Yu. - RUSAKOVA, I. L. Relativistic heavy atom effect on C-13 NMR chemical shifts initiated by adjacent multiple chalcogens. In MAGNETIC RESONANCE IN CHEMISTRY. ISSN 0749-1581, 2018, vol. 56, no. 8, pp. 716-726., Registrované v: WOS
2. [1.1] RUSAKOV, Yury Yu - RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic heavy atom effect on the P-31 NMR parameters of phosphine chalcogenides. Part 1. Chemical shifts. In MAGNETIC RESONANCE IN CHEMISTRY. ISSN 0749-1581, 2018, vol. 56, no. 11, pp. 1061-1073., Registrované v: WOS
3. [1.1] RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic effects in the NMR spectra of compounds containing heavy chalcogens. In MENDELEEV COMMUNICATIONS. ISSN 0959-9436, 2018, vol. 28, no. 1, pp. 1-13., Registrované v: WOS
4. [1.1] VICHA, Jan - KOMOROVSKY, Stanislav - REPISKY, Michal - MAREK, Radek - STRAKA, Michal. Relativistic Spin-Orbit Heavy Atom on the Light Atom NMR Chemical Shifts: General Trends Across the Periodic Table Explained. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 6, pp. 3025-3039., Registrované v: WOS
- ADCA181 KAUPP, Martin - REVIKINE, Roman - MALKINA, Oľga - ARBUZNIKOV, Alexei V. - SCHIMMELPFENNIG, Bernd - MALKIN, Vladimír. Calculation of electronic g-tensors for transition metal complexes using hybrid density functionals and atomic meanfield spin-orbit operators. In Journal of Computational Chemistry, 2002, vol. 23, no. 8, p. 794-803. ISSN 0192-8651.

Citácie:

1. [1.1] KEVORKYANTS, R. - SBOEV, M. N. - CHIZHOV, Yu. V. Electronic-state-driven adsorption of O-2 on a nanocrystalline TiO2 under 'dark'; and UV-irradiation conditions: Ab initio study. In CHEMICAL PHYSICS LETTERS. ISSN 0009-2614, 2018, vol. 698, no., pp. 97-101., Registrované v: WOS
2. [1.1] SAYFUTYAROVA, Elvira R. - CHAN, Garnet Kin-Lic. Electron paramagnetic resonance g-tensors from state interaction spin-orbit coupling density matrix renormalization group. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 18, pp., Registrované v: WOS
3. [1.1] SINGH, Saurabh Kumar - ATANASOV, Mihail - NEESE, Frank. Challenges in Multireference Perturbation Theory for the Calculations of the g-Tensor of First-Row Transition-Metal Complexes. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 9, pp. 4662-4677., Registrované v: WOS
- ADCA182 KAUPP, Martin - REMENYI, Christian - VAARA, Juha - MALKINA, Oľga - MALKIN, Vladimír. Density functional calculations of electronic g-tensors for semiquinone radical anions. The role of hydrogen bonding and substituent effects. In Journal of American Chemical Society, 2002, vol. 124, no. 11, p. 2709-2722.

Citácie:

1. [1.1] JANBAZI, Mehdi - AZAR, Yavar T. - ZIAIE, Farhood. EPR parameters of L-alpha-alanine radicals in aqueous solution: a first-principles study. In MOLECULAR PHYSICS. ISSN 0026-8976, 2018, vol. 116, no. 14, pp. 1795-1803., Registrované v: WOS
2. [1.1] MALISSA, H. - MILLER, R. - BAIRD, D. L. - JAMALI, S. - JOSHI, G. - BURSCH, M. - GRIMME, S. - VAN TOL, J. - LUPTON, J. M. - BOEHME, C. Revealing weak spin-orbit coupling effects on charge carriers in a pi-conjugated polymer. In PHYSICAL REVIEW B. ISSN 2469-9950, 2018, vol. 97, no. 16, pp., Registrované v: WOS
- ADCA183 KAUPP, Martin - MALKINA, Oľga - MALKIN, Vladimír - PYYKKÖ, Pekka. How do spin-orbit-induced heavy-atom effects on NMR chemical shifts function? Validation of a simple analogy to spin-spin coupling by density functional theory (DFT) calculations on some iodo compounds. In Chemistry - A European Journal, 1998, vol. 4, no. 1, p. 118-126. ISSN 0947-6539.

Citácie:

1. [1.1] KOECHER, S. S. - SCHLEKER, P. P. M. - GRAF, M. F. - EICHEL, R.A. - REUTER, K. - GRANWEHR, J. - SCHEURER, Ch. Chemical shift reference scale for Li solid state NMR derived by first-principles DFT calculations. In JOURNAL

OF MAGNETIC RESONANCE. ISSN 1090-7807, 2018, vol. 297, no., pp. 33-41., Registrované v: WOS

2. [1.1] POSADA, Andres F. - MACIAS, Mario A. - MOVILLA, Santiago - PIETRO MISCIONE, Gian - PEREZ, Leon D. - HURTADO, John J. Polymers of epsilon-Caprolactone Using New Copper(II) and Zinc(II) Complexes as Initiators: Synthesis, Characterization and X-Ray Crystal Structures. In POLYMERS. ISSN 2073-4360, 2018, vol. 10, no. 11, pp., Registrované v: WOS

3. [1.1] RUSAKOV, Yu. Yu. - RUSAKOVA, I. L. Relativistic heavy atom effect on C-13 NMR chemical shifts initiated by adjacent multiple chalcogens. In MAGNETIC RESONANCE IN CHEMISTRY. ISSN 0749-1581, 2018, vol. 56, no. 8, pp. 716-726., Registrované v: WOS

4. [1.1] RUSAKOV, Yury Yu - RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic heavy atom effect on the P-31 NMR parameters of phosphine chalcogenides. Part 1. Chemical shifts. In MAGNETIC RESONANCE IN CHEMISTRY. ISSN 0749-1581, 2018, vol. 56, no. 11, pp. 1061-1073., Registrované v: WOS

5. [1.1] RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic effects in the NMR spectra of compounds containing heavy chalcogens. In MENDELEEV COMMUNICATIONS. ISSN 0959-9436, 2018, vol. 28, no. 1, pp. 1-13., Registrované v: WOS

6. [1.1] SANTSCHI, Nico - PITTS, Cody Ross - JELIER, Benson J. - VEREL, Rene. Determining the predominant tautomeric structure of iodine-based group-transfer reagents by O-17 NMR spectroscopy. In BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY. ISSN 1860-5397, 2018, vol. 14, no., pp. 2289-2294., Registrované v: WOS

7. [1.1] SZELL, Patrick M. J. - CAVALLO, Gabriella - TERRANEO, Giancarlo - METRANGOLO, Pierangelo - GABIDULLIN, Bulat - BRYCE, David L. Comparing the Halogen Bond to the Hydrogen Bond by Solid-State NMR Spectroscopy: Anion Coordinated Dimers from 2-and 3-Iodoethynylpyridine Salts. In CHEMISTRY-A EUROPEAN JOURNAL. ISSN 0947-6539, 2018, vol. 24, no. 44, pp. 11364-11376., Registrované v: WOS

8. [1.1] TODISCO, Stefano - SAIELLI, Giacomo - GALLO, Vito - LATRONICO, Mario - RIZZUTI, Antonino - MASTRORILLI, Piero. P-31 and Pt-195 solid-state NMR and DFT studies on platinum(I) and platinum(II) complexes. In DALTON TRANSACTIONS. ISSN 1477-9226, 2018, vol. 47, no. 27, pp. 8884-8891., Registrované v: WOS

9. [1.1] VICHA, Jan - KOMOROVSKY, Stanislav - REPISKY, Michal - MAREK, Radek - STRAKA, Michal. Relativistic Spin-Orbit Heavy Atom on the Light Atom NMR Chemical Shifts: General Trends Across the Periodic Table Explained. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 6, pp. 3025-3039., Registrované v: WOS

10. [1.1] VIESSER, Renan V. - DUCATI, Lucas C. - TORMENA, Claudio F. - AUTSCHBACH, Jochen. The halogen effect on the C-13 NMR chemical shift in substituted benzenes. In PHYSICAL CHEMISTRY CHEMICAL PHYSICS. ISSN 1463-9076, 2018, vol. 20, no. 16, pp. 11247-11259., Registrované v: WOS

ADCA184 KAUPP, Martin - MALKINA, Oľga - MALKIN, Vladimír. The calculation of 17O chemical shielding in transition metal oxo complexes. I. Comparison of DFT and ab initio approaches, and mechanisms of relativity-induced shielding. In Journal of Chemical Physics, 1997, vol. 106, no. 22, p. 9201-9212. (1996: 3.516 - IF, karentované - CCC). (1997 - Current Contents, WOS, SCOPUS, WOS, SCOPUS). ISSN 0021-9606.

Citácie:

1. [1.1] OHLIN, C. Andre - CASEY, William H. O-17 NMR as a Tool in Discrete Metal Oxide Cluster Chemistry. In ANNUAL REPORTS ON NMR SPECTROSCOPY, VOL 94. ISSN 0066-4103, 2018, vol. 94, no., pp. 187-248., Registrované v: WOS

ADCA185 KAUPP, Martin - MALKINA, Oľga - MALKIN, Vladimír. Interpretation of 13C NMR chemical shifts in halomethyl cations. On the importance of spin-orbit coupling and electron correlation. In Chemical Physics Letters, 1997, vol. 265, no. 1-2, p. 55-59. (1997 - Current Contents).

Citácie:

1. [1.1] KOECHER, S. S. - SCHLEKER, P. P. M. - GRAF, M. F. - EICHEL, R.A. - REUTER, K. - GRANWEHR, J. - SCHEURER, Ch. Chemical shift reference scale for Li solid state NMR derived by first-principles DFT calculations. In JOURNAL OF MAGNETIC RESONANCE. ISSN 1090-7807, 2018, vol. 297, no., pp. 33-41., Registrované v: WOS

2. [1.1] RUSAKOV, Yu. Yu. - RUSAKOVA, I. L. Relativistic heavy atom effect on C-13 NMR chemical shifts initiated by adjacent multiple chalcogens. In MAGNETIC RESONANCE IN CHEMISTRY. ISSN 0749-1581, 2018, vol. 56, no. 8, pp. 716-726., Registrované v: WOS

3. [1.1] RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic effects in the NMR spectra of compounds containing heavy chalcogens. In MENDELEEV COMMUNICATIONS. ISSN 0959-9436, 2018, vol. 28, no. 1, pp. 1-13., Registrované v: WOS

4. [1.1] SZELL, Patrick M. J. - CAVALLO, Gabriella - TERRANEO, Giancarlo - METRANGOLO, Pierangelo - GABIDULLIN, Bulat - BRYCE, David L. Comparing the Halogen Bond to the Hydrogen Bond by Solid-State NMR Spectroscopy: Anion Coordinated Dimers from 2-and 3-Iodoethynylpyridine Salts. In CHEMISTRY-A EUROPEAN JOURNAL. ISSN 0947-6539, 2018, vol. 24, no. 44, pp. 11364-11376., Registrované v: WOS

5. [1.1] VICHA, Jan - KOMOROVSKY, Stanislav - REPISKY, Michal - MAREK, Radek - STRAKA, Michal. Relativistic Spin-Orbit Heavy Atom on the Light Atom NMR Chemical Shifts: General Trends Across the Periodic Table Explained. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 6, pp. 3025-3039., Registrované v: WOS

6. [1.1] XIN, Dongyue - JONES, Paul-James - GONNELLA, Nina C. DiCE: Diastereomeric in Silico Chiral Elucidation, Expanded DP4 Probability Theory Method for Diastereomer and Structural Assignment. In JOURNAL OF ORGANIC CHEMISTRY. ISSN 0022-3263, 2018, vol. 83, no. 9, pp. 5035-5043., Registrované v: WOS

ADCA186 KAVECKÝ, Štefan - VALÚCHOVÁ, Jana - ČAPLOVIČOVÁ, Mária - HEISSLER, Stefan - ŠAJGALÍK, Pavol - JANEK, Marián. Nontronites as catalyst for synthesis of carbon nanotubes by catalytic chemical vapor deposition. In Applied Clay Science, 2015, vol. 114, p. 170-178. (2014: 2.467 - IF, Q1 - JCR, 0.918 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] ZEYNALOV, Eldar B. - FRIEDRICH, Joerg F. - TAGIYEV, Dilgam B. - HUSEYNOV, Asgar B. - MAGERRAMOVA, Matanat Ya. - ABDUREHMANOVA, Narmin A. Review on nanostructures from catalytic pyrolysis of gas and liquid carbon sources. In MATERIALS TESTING. ISSN 0025-5300, 2018, vol. 60, no. 7-8, pp. 783-793., Registrované v: WOS

ADCA187 KEDŽUCH, Stanislav - MILKO, Matúš - NOGA, Jozef. Alternative formulation of the matrix elements

in MP2-R12 theory. In *International Journal of Quantum Chemistry*, 2005, vol. 105, no. 6, p. 929-936. ISSN 0020-7608.

Citácie:

1. [1.1] GYORFFY, Werner - WERNER, Hans-Joachim. Analytical energy gradients for explicitly correlated wave functions. II. Explicitly correlated coupled cluster singles and doubles with perturbative triples corrections: CCSD(T)-F12. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 11, pp., Registrované v: WOS
2. [1.1] LASAR, Christian - KLUENER, Thorsten. Explicitly correlated orbital optimized contracted pair correlation methods: Foundations and applications. In *JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY*. ISSN 0219-6336, 2018, vol. 17, no. 4, pp., Registrované v: WOS
3. [1.1] MA, Qianli - WERNER, Hans-Joachim. Explicitly correlated local coupled-cluster methods using pair natural orbitals. In *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*. ISSN 1759-0876, 2018, vol. 8, no. 6, pp., Registrované v: WOS
4. [1.1] MA, Qianli - WERNER, Hans-Joachim. Scalable Electron Correlation Methods. 5. Parallel Perturbative Triples Correction for Explicitly Correlated Local Coupled Cluster with Pair Natural Orbitals. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 1, pp. 198-215., Registrované v: WOS
5. [1.1] PRZYBYTEK, Michal. Dispersion Energy of Symmetry-Adapted Perturbation Theory from the Explicitly Correlated F12 Approach. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 10, pp. 5105-5117., Registrované v: WOS

ADCA188 KELLÖ, Vladimír - NOGA, Jozef - DIERCKSEN, G.H.F. - SADLEJ, A.J. A study of the performance of high-level correlated methods: The energy, dipole moment, and polarizability functions of CO. In *Chemical Physics Letters*, 1988, vol. 152, no. 4-5, p. 387-392. ISSN 0009-2614.

Citácie:

1. [1.1] PANSINI, F. N. N. - DE SOUZA, F. A. L. - CAMPOS, C. T. Molecules under external electric field: On the changes in the electronic structure and validity limits of the theoretical predictions. In *JOURNAL OF COMPUTATIONAL CHEMISTRY*. ISSN 0192-8651, 2018, vol. 39, no. 20, pp. 1561-1567., Registrované v: WOS

ADCA189 KERNER, Lukáš - KICKOVÁ, Anna - FILO, Juraj - KEDŽUCH, Stanislav - PUTALA, Martin. Elucidation of photoisomerization-related structural changes in an acrylamide-bridged binaphthalene-diazene macrocyclic chiroptical switch by experimental electronic circular dichroism spectra simulation: role of dispersion corrections. In *Journal of Physical Chemistry A. Molecules, spectroscopy, kinetics, environment, and general theory*, 2015, vol. 119, p. 8588-8598. (2014: 2.693 - IF, Q2 - JCR, 1.154 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 1089-5639.

Citácie:

1. [1.1] GENG, Wen-Chao - SUN, Hongwei - GUO, Dong-Sheng. Macrocycles containing azo groups: recognition, assembly and application. In *JOURNAL OF INCLUSION PHENOMENA AND MACROCYCLIC CHEMISTRY*. ISSN 1388-3127, 2018, vol. 92, no. 1-2, pp. 1-79., Registrované v: WOS

ADCA190 KLEMENT, Róbert - KRAXNER, Jozef - LIŠKA, Marek. Spectroscopic analysis of iron doped glasses with composition close to the E-glass: A preliminary study. In *Ceramics-Silikáty*, 2009, vol. 53, no. 3, p. 180-183. (2008: 0.644 - IF). ISSN 0862-5468.

Citácie:

1. [1.1] MANDAL, Ashis K. - MANDAL, B. - ILLATH, Kavya - AJITHKUMAR, T. G. - HALDER, A. - SINHA, P. K. - SEN, Ranjan. Preparation of colourless phosphate glass by stabilising higher Fe[II] in microwave heating. In *SCIENTIFIC REPORTS*. ISSN 2045-2322, 2018, vol. 8, no., pp., Registrované v: WOS
2. [1.1] MANDAL, Ashis K. - SEN, Ranjan. Preservation of higher Fe[III] content in borosilicate glass by microwave irradiation in air. In *MATERIALS RESEARCH BULLETIN*. ISSN 0025-5408, 2018, vol. 108, no., pp. 156-162., Registrované v: WOS
3. [1.1] PATHAK, M. S. - GOPAL, N. O. - SINGH, N. - MOHAPATRA, M. - RAO, J. L. - LEE, Jung-Kul - SINGH, Vijay. Synthesis and investigations on correlation between EPR and optical properties of Fe doped Li₂SiO₃. In *JOURNAL OF NON-CRYSTALLINE SOLIDS*. ISSN 0022-3093, 2018, vol. 500, no., pp. 266-271., Registrované v: WOS

ADCA191 KLOPPER, Wim - NOGA, Jozef. Accurate quantum-chemical prediction of enthalpies of formation of small molecules in the gas phase. In *ChemPhysChem*, 2003, vol. 4, no. 1, p. 32-48. ISSN 1439-7641.

Citácie:

1. [1.1] VARANDAS, Antonio J. C. Straightening the Hierarchical Staircase for Basis Set Extrapolations: A Low-Cost Approach to High-Accuracy Computational Chemistry. In *ANNUAL REVIEW OF PHYSICAL CHEMISTRY*, VOL 69. ISSN 0066-426X, 2018, vol. 69, no., pp. 177-203., Registrované v: WOS

ADCA192 KLOPPER, Wim - NOGA, Jozef - KOCH, Henrik - HELGAKER, Trygve. Multiple basis sets in calculations of triples corrections in coupled-cluster theory. In *Theoretical Chemistry Accounts*, 1997, vol. 97, no. 1-4, p. 164-176.

Citácie:

1. [1.1] KESHARWANI, Manoj K. - SYLVETSKY, Nitai - KOEHN, Andreas - TEW, David P. - MARTIN, Jan M. L. Do CCSD and approximate CCSD-F12 variants converge to the same basis set limits? The case of atomization energies. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 15, pp., Registrované v: WOS
2. [1.1] LIU, Lei - LEE, Wes - YUAN, Mingbin - GUTIERREZ, Osvaldo. Mechanisms of Bisphosphine Iron-Catalyzed C(SP²)-C(SP³) Cross-Coupling Reactions: Inner-Sphere or Outer-Sphere Arylation? In *COMMENTS ON INORGANIC CHEMISTRY*. ISSN 0260-3594, 2018, vol. 38, no. 6, pp. 210-237., Registrované v: WOS
3. [1.1] YOKOGAWA, D. Coupled Cluster Theory Combined with Reference Interaction Site Model Self-Consistent Field Explicitly Including Spatial Electron Density Distribution. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 5, pp. 2661-2666., Registrované v: WOS

ADCA193 KOETTGEN, Julius - SCHMIDT, Peter C. - BUČKO, Tomáš - MARTIN, Manfred. Ab initio

calculation of the migration free energy of oxygen diffusion in pure and samarium-doped ceria. In *Physical Review B*, 2018, vol. 97, no. 2, art. no. 024305. (2017: 3.813 - IF, Q2 - JCR, 1.176 - SJR, Q1 - SJR, karentované - CCC). (2018 - Current Contents, WOS, SCOPUS). ISSN 1550-235X.

Citácie:

1. [1.1] GRIESHAMMER, Steffen. Influence of the lattice constant on defects in cerium oxide. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 30, pp. 19792-19799., Registrované v: WOS

ADCA194 KOMADEL, Peter - MADEJOVÁ, Jana - STUCKI, Joseph W. Reduction and reoxidation of nontronite: Questions of reversibility. In *Clays and Clay Minerals*, 1995, vol. 43, no. 1, p. 105-110. ISSN 0009-8604.

Citácie:

1. [1.1] FERNANDEZ, A. M. - KAUFHOLD, S. - SANCHEZ-LEDESMA, D. M. - REY, J. J. - MELON, A. - ROBREDO, L. M. - FERNANDEZ, S. - LABAJO, M. A. - CLAVERO, M. A. Evolution of the THC conditions in the FEBEX in situ test after 18 years of experiment: Smectite crystallochemical modifications after interactions of the bentonite with a C-steel heater at 100 degrees C. In *APPLIED GEOCHEMISTRY*. ISSN 0883-2927, 2018, vol. 98, no., pp. 152-171., Registrované v: WOS
2. [1.1] KISIEL, Marta - SKIBA, Michal - SKONECZNA, Magdalena - MAJ-SZELIGA, Katarzyna - BLACHOWSKI, Artur. Weathering of glauconite in an alkaline environment A case study from Krakow area, Poland. In *CATENA*. ISSN 0341-8162, 2018, vol. 171, no., pp. 541-551., Registrované v: WOS
3. [1.1] ROMANOV, Vyacheslav - MYSHAKIN, Evgeniy M. Experimental Studies: Clay Swelling. In *GREENHOUSE GASES AND CLAY MINERALS: ENLIGHTENING DOWN-TO-EARTH ROAD MAP TO BASIC SCIENCE OF CLAY-GREENHOUSE GAS INTERFACES*. ISSN 1865-3529, 2018, vol., no., pp. 125-145., Registrované v: WOS

ADCA195 KOMADEL, Peter - BUJDÁK, Juraj - MADEJOVÁ, Jana - ŠUCHA, Vladimír - ELSASS, Françoise. Effect of non-swelling layers on the dissolution of reduced-charge montmorillonite in hydrochloric acid. In *Clay Minerals*, 1996, vol. 31, no. 3, p. 333-345. ISSN 0009-8558.

Citácie:

1. [1.1] ALVER, Burcu Erdogan. Hydrogen adsorption on natural and sulphuric acid treated sepiolite and bentonite. In *INTERNATIONAL JOURNAL OF HYDROGEN ENERGY*. ISSN 0360-3199, 2018, vol. 43, no. 2, pp. 831-838., Registrované v: WOS
2. [1.1] ANTONIO CECILIA, Juan - PARDO, Laura - POZO, Manuel - BELLIDO, Eva - FRANCO, Francisco. Microwave-Assisted Acid Activation of Clays Composed of 2:1 Clay Minerals: A Comparative Study. In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 9, pp., Registrované v: WOS
3. [1.1] DUTTA, Dipak Kumar. Clay mineral catalysts. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS*, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 289-329., Registrované v: WOS
4. [1.1] TOHDEE, Kanogwan - KAEWSICHAN, Lupon - ASADULLAH. Enhancement of adsorption efficiency of heavy metal Cu(II) and Zn(II) onto cationic surfactant modified bentonite. In *JOURNAL OF ENVIRONMENTAL CHEMICAL ENGINEERING*. ISSN 2213-3437, 2018, vol. 6, no. 2, pp. 2821-2828., Registrované v: WOS

ADCA196 KOMADEL, Peter - MADEJOVÁ, Jana - JANEK, Marián - GATES, W.P. - KIRKPATRICK, R.J. - STUCKI, Joseph W. Dissolution of hectorite in inorganic acids. In *Clays and Clay Minerals*, 1996, vol. 44, no. 2, p. 228-236. ISSN 0009-8604.

Citácie:

1. [1.1] CHIU, Hsien-Lung - LIAO, Ying-Chih - PAN, Guan-Ting - CHONG, Siewhui. Hybrid nanocomposite film with enhanced moisture barrier properties. In *JOURNAL OF THE TAIWAN INSTITUTE OF CHEMICAL ENGINEERS*. ISSN 1876-1070, 2018, vol. 83, no., pp. 168-173., Registrované v: WOS
2. [1.1] JOZEFACIUK, G. - SZATANIK-KLOC, A. - AMBROZEWICZ-NITA, A. The surface area of zeolite-amended soils exceeds the sum of the inherent surface areas of soil and zeolite. In *EUROPEAN JOURNAL OF SOIL SCIENCE*. ISSN 1351-0754, 2018, vol. 69, no. 5, pp. 787-790., Registrované v: WOS
3. [1.1] KHABBOUCHI, M. - HOSNI, K. - SRASRA, E. Physico-Chemical Characterization of Modified Tunisian Kaolin by Phosphoric Acid. In *SURFACE ENGINEERING AND APPLIED ELECTROCHEMISTRY*. ISSN 1068-3755, 2018, vol. 54, no. 2, pp. 219-226., Registrované v: WOS

ADCA197 KOMADEL, Peter - JANEK, Marián - MADEJOVÁ, Jana - WEEKES, A. - BREEN, Christopher. Acidity and catalytic activity of mildly acid-treated Mg-rich montmorillonite and hectorite. In *Journal of the Chemical Society-Faraday Transactions*, 1997, vol. 93, no. 23, p. 4207-4210.

Citácie:

1. [1.1] AL-ESSA, Khansaa. Activation of Jordanian Bentonite by Hydrochloric Acid and Its Potential for Olive Mill Wastewater Enhanced Treatment. In *JOURNAL OF CHEMISTRY*. ISSN 2090-9063, 2018, vol., no., pp., Registrované v: WOS
2. [1.1] DUTTA, Dipak Kumar. Clay mineral catalysts. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS*, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 289-329., Registrované v: WOS
3. [1.1] PHUKAN, Ankana - BHORODWAJ, Siddhartha Kumar - SHARMA, Podma Pollov - DUTTA, Dipak Kumar. Mesoporous aluminosilicate: efficient and reusable catalysts for esterification of sec-butanol with acetic acid. In *JOURNAL OF POROUS MATERIALS*. ISSN 1380-2224, 2018, vol. 25, no. 1, pp. 129-136., Registrované v: WOS
4. [1.1] ZOPE, Indraneel Suhas. Literature Review. In *FIRE RETARDANCY BEHAVIOR OF POLYMER/CLAY NANOCOMPOSITES*. ISSN 2190-5053, 2018, vol., no., pp. 13-39., Registrované v: WOS

ADCA198 KOMADEL, Peter - MADEJOVÁ, Jana - BUJDÁK, Juraj. Preparation and properties of reduced-charge smectites - A review. In *Clays and Clay Minerals*, 2005, vol. 53, no. 4, p. 313-334. (2004: 1.116 - IF, karentované - CCC). (2005 - Current Contents). ISSN 0009-8604.

Citácie:

1. [1.1] BODART, Philippe R. - DELMOTTE, L. - RIGOLET, S. - BRENDLE, J. - GOUGEON, Régis D. Li-7[F-19] TEDOR NMR to observe the lithium migration in heated montmorillonite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 157, no.,

pp. 204-211., Registrované v: WOS

2. [1.1] DING, Fan - GAO, Manglai - WANG, Jie - SHEN, Tao - ZANG, Weili. Tuning wettability by controlling the layer charge and structure of organo-vermiculites. In *JOURNAL OF INDUSTRIAL AND ENGINEERING CHEMISTRY*. ISSN 1226-086X, 2018, vol. 57, no., pp. 304-312., Registrované v: WOS

3. [1.1] EBINA, Takeo. Development of Clay-Based Films. In *CHEMICAL RECORD*. ISSN 1527-8999, 2018, vol. 18, no. 7-8, pp. 1020-1032., Registrované v: WOS

4. [1.1] HUANG, Xue - YIN, Guoqiang - FENG, Guangzhu. Organic modification of montmorillonite and effect of catalytic selectivity on the dimerization of unsaturated fatty acid. In *TURKISH JOURNAL OF CHEMISTRY*. ISSN 1300-0527, 2018, vol. 42, no. 1, pp. 50-62., Registrované v: WOS

5. [1.1] SCHIEBEL, Korbinian - JORDAN, Guntram - KAESTNER, Anders - SCHILLINGER, Burkhard - GEORGII, Robert - HESS, Kai-Uwe - BOEHNKE, Sandra - SCHMAHL, Wolfgang W. Effects of heat and cyclic reuse on the properties of bentonite-bonded sand. In *EUROPEAN JOURNAL OF MINERALOGY*. ISSN 0935-1221, 2018, vol. 30, no. 6, pp. 1115-1125., Registrované v: WOS

6. [1.1] TOSCA, Nicholas J. - WRIGHT, V. Paul. Diagenetic pathways linked to labile Mg-clays in lacustrine carbonate reservoirs: a model for the origin of secondary porosity in the Cretaceous pre-salt Barra Velha Formation, offshore Brazil. In *RESERVOIR QUALITY OF CLASTIC AND CARBONATE ROCKS: ANALYSIS, MODELLING AND PREDICTION*. ISSN 0305-8719, 2018, vol. 435, no., pp. 33-46., Registrované v: WOS

ADCA199 KOMADEL, Peter - MADEJOVÁ, Jana - STUCKI, Joseph W. Structural Fe(III) reduction in smectites. In *Applied Clay Science*, 2006, vol. 34, no. 1-4, p. 88-94. (2005: 1.324 - IF, karentované - CCC). (2006 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] FERNANDEZ, A. M. - KAUFHOLD, S. - SANCHEZ-LEDESMA, D. M. - REY, J. J. - MELON, A. - ROBREDO, L. M. - FERNANDEZ, S. - LABAJO, M. A. - CLAVERO, M. A. Evolution of the THC conditions in the FEBEX in situ test after 18 years of experiment: Smectite crystallochemical modifications after interactions of the bentonite with a C-steel heater at 100 degrees C. In *APPLIED GEOCHEMISTRY*. ISSN 0883-2927, 2018, vol. 98, no., pp. 152-171., Registrované v: WOS

2. [1.1] SHAKERI, Sirous - ABTAHI, Seyed A. Potassium forms in calcareous soils as affected by clay minerals and soil development in Kohgiluyeh and Boyer-Ahmad Province, Southwest Iran. In *JOURNAL OF ARID LAND*. ISSN 1674-6767, 2018, vol. 10, no. 2, pp. 217-232., Registrované v: WOS

3. [1.1] YUAN, Songhu - LIU, Xixiang - LIAO, Wenjuan - ZHANG, Peng - WANG, Xiaoming - TONG, Man. Mechanisms of electron transfer from structural Fe(II) in reduced nontronite to oxygen for production of hydroxyl radicals. In *GEOCHIMICA ET COSMOCHIMICA ACTA*. ISSN 0016-7037, 2018, vol. 223, no., pp. 422-436., Registrované v: WOS

ADCA200 KOMADEL, Peter - MADEJOVÁ, Jana - STUCKI, Joseph W. Partial stabilization of Fe(II) in reduced ferruginous smectite by Li fixation. In *Clays and Clay Minerals*, 1999, vol. 47, no. 4, p. 458-465. (1998: 1.010 - IF).

Citácie:

1. [1.1] ALAZIGHA, Dennis Pere - INDRARATNA, Buddhima - VINOD, Jayan S. - HEITOR, Ana. Mechanisms of stabilization of expansive soil with lignosulfonate admixture. In *TRANSPORTATION GEOTECHNICS*. ISSN 2214-3912, 2018, vol. 14, no., pp. 81-92., Registrované v: WOS

2. [1.1] PELAYO, M. - MARCO, J. F. - FERNANDEZ, A. M. - VERGARA, L. - MELON, A. M. - PEREZ DEL VILLAR, L. Infrared and Mossbauer spectroscopy of Fe-rich smectites from Morron de Mateo bentonite deposit (Spain). In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 1, pp. 17-28., Registrované v: WOS

ADCA201 KOMOROVSKÝ, Stanislav - REPISKÝ, Michal - RUUD, Kenneth - MALKINA, Olga - MALKIN, Vladimír. Four-component relativistic density functional theory calculations of NMR shielding tensors for paramagnetic systems. In *Journal of Physical Chemistry A. Molecules, spectroscopy, kinetics, environment, and general theory*, 2013, vol. 117, no. 51, p. 14209-14219. (2012: 2.771 - IF, 1.494 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 1089-5639.

Citácie:

1. [1.1] CHYBA, Jan - NOVAK, Martin - MUNZAROVA, Petra - NOVOTNY, Jan - MAREK, Radek. Through-Space Paramagnetic NMR Effects in Host-Guest Complexes: Potential Ruthenium(III) Metallodrugs with Macrocyclic Carriers. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 15, pp. 8735-8747., Registrované v: WOS

2. [1.1] MONDAL, Arobindo - GAULTOIS, Michael W. - PELL, Andrew J. - IANNUZZI, Marcella - GREY, Clare P. - HUTTER, Jurg - KAUPP, Martin. Large-Scale Computation of Nuclear Magnetic Resonance Shifts for Paramagnetic Solids Using CP2K. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 1, pp. 377-394., Registrované v: WOS

3. [1.1] PAGOLA, Gabriel I. - LARSEN, Martin A. B. - FERRARO, Marta - SAUER, Stephan P. A. The influence of relativistic effects on nuclear magnetic resonance spin-spin coupling constant polarizabilities of H₂O₂, H₂S₂, H₂Se₂, and H₂Te₂. In *JOURNAL OF COMPUTATIONAL CHEMISTRY*. ISSN 0192-8651, 2018, vol. 39, no. 31, pp. 2589-2600., Registrované v: WOS

4. [1.1] RUSAKOV, Yury Yu - RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic heavy atom effect on the P-31 NMR parameters of phosphine chalcogenides. Part 1. Chemical shifts. In *MAGNETIC RESONANCE IN CHEMISTRY*. ISSN 0749-1581, 2018, vol. 56, no. 11, pp. 1061-1073., Registrované v: WOS

ADCA202 KOMOROVSKÝ, Stanislav - REPISKÝ, Michal - MALKINA, Olga - MALKIN, Vladimír. Fully relativistic calculations of NMR shielding tensors using restricted magnetically balanced basis and gauge including atomic orbitals. In *Journal of Chemical Physics*, 2010, vol. 132, no. 15, p. 154101-1-154101-8. (2009: 3.093 - IF, karentované - CCC). (2010 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] HAYAMI, Masao - SEINO, Junji - NAKAI, Hiromi. Gauge-origin independent formalism of two-component relativistic framework based on unitary transformation in nuclear magnetic shielding constant. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 11, pp., Registrované v: WOS

- ADCA203 KOMOROVSKÝ, Stanislav - REPISKÝ, Michal - MALKINA, Oľga - MALKIN, Vladimír - MALKIN, Irina - KAUPP, Martin. Resolution of identity Dirac-Kohn-Sham method using the large component only: Calculations of g-tensor and hyperfine tensor. In *Journal of Chemical Physics*, 2006, vol. 124, no. 8, p. 084108-1-084108-8. (2005: 3.138 - IF). ISSN 0021-9606.

Citácie:

- [1.1] SAYFUTYAROVA, Elvira R. - CHAN, Garnet Kin-Lic. Electron paramagnetic resonance g-tensors from state interaction spin-orbit coupling density matrix renormalization group. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 18, pp., Registrované v: WOS

- ADCA204 KOMOROVSKÝ, Stanislav - REPISKÝ, Michal - MALKINA, Oľga - MALKIN, Vladimír - MALKIN-ONDÍK, Irina - KAUPP, Martin. A fully relativistic method for calculation of nuclear magnetic shielding tensors with a restricted magnetically balanced basis in the framework of the matrix Dirac-Kohn-Sham equation. In *Journal of Chemical Physics*, 2008, vol. 128, no. 10, p. 104101-1-104101-15. (2007: 3.044 - IF, karentované - CCC). (2008 - Current Contents). ISSN 0021-9606.

Citácie:

- [1.1] AUCAR, Gustavo A. - MELO, Juan I. - AGUSTIN AUCAR, Ignacio - MALDONADO, Alejandro F. Foundations of the LRESC model for response properties and some applications. In *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY*. ISSN 0020-7608, 2018, vol. 118, no. 1, pp., Registrované v: WOS
- [1.1] CHENG, Lan - WANG, Fan - STANTON, John F. - GAUSS, Juergen. Perturbative treatment of spin-orbit-coupling within spin-free exact two-component theory using equation-of-motion coupled-cluster methods. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 4, pp., Registrované v: WOS
- [1.1] FIELD-THEODORE, Terri E. - OLEJNICZAK, Malgorzata - JASZUNSKI, Michal - WILSON, David J. D. NMR shielding constants in group 15 trifluorides. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 35, pp. 23025-23033., Registrované v: WOS
- [1.1] KOECHER, S. S. - SCHLEKER, P. P. M. - GRAF, M. F. - EICHEL, R.A. - REUTER, K. - GRANWEHR, J. - SCHEURER, Ch. Chemical shift reference scale for Li solid state NMR derived by first-principles DFT calculations. In *JOURNAL OF MAGNETIC RESONANCE*. ISSN 1090-7807, 2018, vol. 297, no., pp. 33-41., Registrované v: WOS
- [1.1] LIU, Junzi - CHENG, Lan. An atomic mean-field spin-orbit approach within exact two-component theory for a non-perturbative treatment of spin-orbit coupling. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 14, pp., Registrované v: WOS
- [1.1] REYNOLDS, Ryan D. - YANAI, Takeshi - SHIOZAKI, Toru. Large-scale relativistic complete active space self-consistent field with robust convergence. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 1, pp., Registrované v: WOS
- [1.1] RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic effects in the NMR spectra of compounds containing heavy chalcogens. In *MENDELEEV COMMUNICATIONS*. ISSN 0959-9436, 2018, vol. 28, no. 1, pp. 1-13., Registrované v: WOS

- ADCA205 KONEČNÝ, Lukáš - KÁDEK, Marius - KOMOROVSKÝ, Stanislav - MALKINA, Oľga - RUUD, Kenneth - REPISKÝ, Michal. Acceleration of relativistic electron dynamics by means of X2C transformation: Application to the calculation of nonlinear optical properties. In *Journal of Chemical Theory and Computation*, 2016, vol. 12, no., p. 5823-5833. (2015: 5.301 - IF, Q1 - JCR, 2.702 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 1549-9618.

Citácie:

- [1.1] GOINGS, Joshua J. - EGIDI, Franco - LI, Xiaosong. Current development of noncollinear electronic structure theory. In *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY*. ISSN 0020-7608, 2018, vol. 118, no. 1, pp., Registrované v: WOS
- [1.1] GOINGS, Joshua J. - LESTRANGE, Patrick J. - LI, Xiaosong. Real-time time-dependent electronic structure theory. In *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*. ISSN 1759-0876, 2018, vol. 8, no. 1, pp., Registrované v: WOS
- [1.1] KASPER, Joseph M. - LESTRANGE, Patrick J. - STETINA, Torin F. - LIA, Xiaosong. Modeling L-2,L-3-Edge X-ray Absorption Spectroscopy with Real-Time Exact Two-Component Relativistic Time-Dependent Density Functional Theory. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 4, pp. 1998-2006., Registrované v: WOS
- [1.1] LIU, Wenjian - XIAO, Yunlong. Relativistic time-dependent density functional theories. In *CHEMICAL SOCIETY REVIEWS*. ISSN 0306-0012, 2018, vol. 47, no. 12, pp. 4481-4509., Registrované v: WOS
- [1.1] NORMAN, Patrick - DREUW, Andreas. Simulating X-ray Spectroscopies and Calculating Core-Excited States of Molecules. In *CHEMICAL REVIEWS*. ISSN 0009-2665, 2018, vol. 118, no. 15, pp. 7208-7248., Registrované v: WOS
- [1.1] PETRONE, Alessio - WILLIAMS-YOUNG, David B. - SUN, Shichao - STETINA, Torin F. - LI, Xiaosong. An efficient implementation of two-component relativistic density functional theory with torque-free auxiliary variables. In *EUROPEAN PHYSICAL JOURNAL B*. ISSN 1434-6028, 2018, vol. 91, no. 7, pp., Registrované v: WOS

- ADCA206 KONETSCHNY, Christoph - GALUSEK, Dušan - RESCHKE, S. - FASEL, Claudia - RIEDEL, Ralf. Dense silicon carbonitride ceramics by pyrolysis of cross-linked and warm pressed polysilazane powders. In *Journal of the European Ceramic Society*, 1999, vol. 19, no. 16, p. 2789-2796. ISSN 0955-2219.

Citácie:

- [1.1] PRATAVIERA, Rogerio - PESSAN, Luiz Antonio - FELIX CARVALHO, Antonio Jose. Characterization of thermally crosslinkable polyester films by thermomechanical analysis: a versatile and very sensitive technique for the evaluation of low crosslinking degree in polymers. In *POLYMER INTERNATIONAL*. ISSN 0959-8103, 2018, vol. 67, no. 8, pp. 1011-1015., Registrované v: WOS
- [1.1] WANG, Qi - YANG, Mei - XIAO, Jiusan - JIAO, Shuqiang - ZHU, Hongmin. Synthesis, characterization and sintering of Si-C-N nano-powders via sodium reduction in liquid ammonia. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN

0955-2219, 2018, vol. 38, no. 4, pp. 1219-1226., Registrované v: WOS

- ADCA207 KORENKO, Michal - VASKOVÁ, Zuzana - PRISČÁK, Jozef - ŠIMKO, František - AMBROVÁ, Marta - SHI, Zhongning. Density, viscosity and electrical conductivity of the molten cryolite electrolytes (Na₃AlF₆-SiO₂) for solar grade silicon (Si-SoG) electrowinning. In *Silicon*, 2015, vol. 7, no. 3, p. 261-267. (2014: 1.069 - IF, Q3 - JCR, 0.313 - SJR, Q3 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 1876-990X.

Citácie:

1. [1.1] KUBIKOVA, Blanka - MLYNARIKOVA, Jarmila - BENES, Ondrej - MIKSIKOVA, Eva - PRISCAK, Jozef - TOSOLIN, Alberto - BOCA, Miroslav. Physico-chemical properties of the system (LiF-NaF)(eut)-LaF₃ Phase equilibria, density and volume properties, electrical conductivity and surface tension. In *JOURNAL OF MOLECULAR LIQUIDS*. ISSN 0167-7322, 2018, vol. 268, no., pp. 754-761., Registrované v: WOS

- ADCA208 KORENKO, Michal - STRAKA, Martin - SZATMÁRY, Lórant - AMBROVÁ, Marta - UHLÍŘ, J. Electrochemical separation of uranium in the molten system LiF-NaF-KF-UF₄. In *Journal of Nuclear Materials*, 2013, vol. 440, no. 1-3, p. 332-337. (2012: 1.211 - IF, 0.856 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 0022-3115.

Citácie:

1. [1.1] AGARWAL, Rahul - SHARMA, Manoj Kumar. Selective Electrochemical Separation and Recovery of Uranium from Mixture of Uranium(VI) and Lanthanide(III) Ions in Aqueous Medium. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 17, pp. 10984-10992., Registrované v: WOS

2. [1.1] HAN, Dong - SHE, ChangFeng - PENG, Jia - JIANG, Feng - YANG, Xu - PENG, Hao - YANG, Yang - ZHENG, Haiyang - WANG, Xianbin - XU, Qianhui - WANG, Chenyang - ZHU, Tiejian - LUO, Yan - HUANG, Wei - GONG, Yu - LI, Qingnuan. Electrochemical Behavior of UO₂F₂ and Its Electrodeposition from UO₂F₂-FLiNaK Melt. In *JOURNAL OF THE ELECTROCHEMICAL SOCIETY*. ISSN 0013-4651, 2018, vol. 165, no. 7, pp. D301-D306., Registrované v: WOS

3. [1.1] HELAL, A. S. - MAZARIO, E. - MAYORAL, A. - DECORSE, P. - LOSNO, R. - LION, C. - AMMAR, S. - HEMADI, M. Highly efficient and selective extraction of uranium from aqueous solution using a magnetic device: succinyl-beta-cyclodextrin-APTES@maghemite nanoparticles. In *ENVIRONMENTAL SCIENCE-NANO*. ISSN 2051-8153, 2018, vol. 5, no. 1, pp. 158-168., Registrované v: WOS

4. [1.1] PENG, Hao - SHEN, Miao - ZUO, Yong - FU, Haiying - XIE, Leidong. Chemical and electrochemical studies on the solubility of UO₂ in molten FLiNaK with ZrF₄ additive. In *JOURNAL OF NUCLEAR MATERIALS*. ISSN 0022-3115, 2018, vol. 510, no., pp. 256-264., Registrované v: WOS

5. [1.1] STIKA, M. - PADILLA, S. - JARRELL, J. - BLUE, T. - CAO, L. R. - SIMPSON, M. Thin-Layer Electrodeposition of Uranium Metal from Molten LiCl-KCl. In *JOURNAL OF THE ELECTROCHEMICAL SOCIETY*. ISSN 0013-4651, 2018, vol. 165, no. 3, pp. D135-D141., Registrované v: WOS

6. [1.1] ZHANG, Milin - WANG, Pu - ZHANG, Yiming - JI, Debin - YAN, Yongde - SHI, Weiqun - HUANG, Qing - DU, Shiyu. New formulation for reduction potentials of (Cu, Ni, Al, Zn)-lanthanide alloys Implications for electrolysis-based pyroprocessing of spent nuclear fuel. In *ELECTROCHEMISTRY COMMUNICATIONS*. ISSN 1388-2481, 2018, vol. 93, no., pp. 180-182., Registrované v: WOS

- ADCA209 KOSA, Ladislav - MACKOVÁ, Iveta - PROKS, Ivo - PRITULA, Ondrej - SMRČOK, Ľubomír - BOČA, Miroslav - RUNDLÖF, Hakan. Phase transitions of K₂TaF₇ within 680-800 °C. In *Central European Journal of Chemistry*, 2008, vol. 6, no. 1, p. 27-32. (2007: 0.754 - IF). (2008 - WOS, SCOPUS). ISSN 1895-1066.

Citácie:

1. [1.1] LEE, YoungJun - YOO, BungUk - NERSISYAN, Hayk H. - LEE, Jong-Hyeon. Temperature and Concentration Dependencies of LiF-NaF-K₂TaF₇ Phase Equilibria and Effects on Ta Electrodeposition Layer. In *JOURNAL OF THE ELECTROCHEMICAL SOCIETY*. ISSN 0013-4651, 2018, vol. 165, no. 10, pp. D432-D438., Registrované v: WOS

- ADCA210 KOVALČÍKOVÁ, Alexandra - SEDLÁČEK, Jaroslav - LENCĚŠ, Zoltán - BYSTRICKÝ, Roman - DUSZA, Ján - ŠAJGALÍK, Pavol. Oxidation resistance of SiC ceramics prepared by different processing routes. In *Journal of the European Ceramic Society*, 2016, vol. 36, p. 3783-3793. (2015: 2.933 - IF, Q1 - JCR, 1.150 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0955-2219.

Citácie:

1. [1.1] CHENG, Chunyu - LIE, Hejun - FU, Qiangang - GUO, Liping. Effect of Al₂O₃ on the densification and oxidation behavior of SiC coating for carbon/carbon composites. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 11, pp. 12702-12708., Registrované v: WOS

2. [1.1] CHO, Tae-Young - MALIK, Rohit - KIM, Young-Wook - KIM, Kwang Joo. Electrical and mechanical properties of pressureless sintered SiC-Ti₂CN composites. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 9, pp. 3064-3072., Registrované v: WOS

3. [1.1] SEO, Yu-Kwang - EOM, Jung-Hye - KIM, Young-Wook. Process-tolerant pressureless-sintered silicon carbide ceramics with alumina-yttria-calcia-strontia. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 2, pp. 445-452., Registrované v: WOS

4. [1.1] SUN, Rongyan - YANG, Xu - OHKUBO, Yuji - ENDO, Katsuyoshi - YAMAMURA, Kazuya. Optimization of Gas Composition Used in Plasma Chemical Vaporization Machining for Figuring of Reaction-Sintered Silicon Carbide with Low Surface Roughness. In *SCIENTIFIC REPORTS*. ISSN 2045-2322, 2018, vol. 8, no., pp., Registrované v: WOS

5. [1.2] XU, Chengying. Effect of processing conditions on electric and dielectric properties of polymer-derived sic ceramics. In *Ceramic Transactions*. ISSN 10421122, 2018-01-01, 265, pp. 165-174., Registrované v: SCOPUS

- ADCA211 KOVALČÍKOVÁ, Alexandra - DUSZA, Ján - ŠAJGALÍK, Pavol. Thermal shock resistance and fracture toughness of liquid-phase-sintered SiC-based ceramics. In *Journal of the European Ceramic*

Society, 2009, vol. 29, p. 2387-2394. (2008: 1.580 - IF, karentované - CCC). (2009 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] BAITALIK, Sanchita - KAYAL, Nijhuma. Dispersion of SiC powder suspension in mullite sol and influence on properties of sintered ceramics. In *INTERNATIONAL JOURNAL OF APPLIED CERAMIC TECHNOLOGY*. ISSN 1546-542X, 2018, vol. 15, no. 2, pp. 426-437., Registrované v: WOS
2. [1.1] CHEN, Junjun - CHEN, Jian - CHEN, Zhongming - LIU, Xuejian - HUANG, Zhengren - HUANG, Yihua. Potential-current characteristics in SiC/ZrB₂ composite ceramics. In *Journal of the European Ceramic Society*. ISSN 09552219, 2018-06-01, 38, 6, pp. 2477-2485., Registrované v: WOS
3. [1.1] MA, Weiquan - HONG, Tao - XIE, Tian - WANG, Fengxia - LUO, Bin - ZHOU, Jie - YANG, Yang - ZHU, Huacheng - HUANG, Kama. Simulation and Analysis of Oleic Acid Pretreatment for Microwave-Assisted Biodiesel Production. In *PROCESSES*. ISSN 2227-9717, 2018, vol. 6, no. 9, pp., Registrované v: WOS
4. [1.1] YAO, Y. - CHAI, H. W. - LI, C. - BIE, B. X. - XIAO, X. H. - HUANG, J. Y. - QI, M. L. - LUO, S. N. Deformation and damage of sintered low-porosity aluminum under planar impact: microstructures and mechanisms. In *JOURNAL OF MATERIALS SCIENCE*. ISSN 0022-2461, 2018, vol. 53, no. 6, pp. 4582-4597., Registrované v: WOS

ADCA212 KRAKNER, Jozef - LIŠKA, Marek - KLEMENT, Róbert - CHROMČÍKOVÁ, Mária. Surface tension of borosilicate melts with the composition close to the E-glass. In *Ceramics-Silikáty*, 2009, vol. 53, no. 2, p. 141-143. (2008: 0.644 - IF). ISSN 0862-5468.

Citácie:

1. [1.1] MIR, Anamul H. - HINKS, J. A. - DELAYE, Jean-Marc - PEUGET, Sylvain - DONNELLY, S. E. Xenon solubility and formation of supercritical xenon precipitates in glasses under non-equilibrium conditions. In *SCIENTIFIC REPORTS*. ISSN 2045-2322, 2018, vol. 8, no., pp., Registrované v: WOS

ADCA213 KŘÍSTKOVÁ, Anežka - ASHER, James Richard - MALKIN, Vladimír - MALKINA, Oľga. Indirect nuclear (15)N-(15)N scalar coupling through a hydrogen bond: dependence on structural parameters studied by quantum chemistry tools. In *Journal of Physical Chemistry A. Molecules, spectroscopy, kinetics, environment, and general theory*, 2013, vol. 117, no. 38, p. 9235-9244. (2012: 2.771 - IF, 1.494 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 1089-5639.

Citácie:

1. [1.1] SHENDEROVICH, Ilya G. Simplified calculation approaches designed to reproduce the geometry of hydrogen bonds in molecular complexes in aprotic solvents. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 12, pp., Registrované v: WOS

ADCA214 KŘÍSTKOVÁ, Anežka - KOMOROVSKÝ, Stanislav - REPISKÝ, Michal - MALKIN, Vladimír - MALKINA, Oľga. Relativistic four-component calculations of indirect nuclear spin-spin couplings with efficient evaluation of the exchange-correlation response kernel. In *Journal of Chemical Physics*, 2015, vol. 142, no. 11, p. 114102-1-114102-10. (2014: 2.952 - IF, Q1 - JCR, 1.386 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] JAKUBOWSKA, Katarzyna - PECUL, Magdalena - JASZUNSKI, Michal. Spin-spin coupling constants in HC=CX₃ molecules; X=C, Si, Ge, Sn and Pb. In *THEORETICAL CHEMISTRY ACCOUNTS*. ISSN 1432-881X, 2018, vol. 137, no. 3, pp., Registrované v: WOS
2. [1.1] SHENDEROVICH, Ilya G. Simplified calculation approaches designed to reproduce the geometry of hydrogen bonds in molecular complexes in aprotic solvents. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 12, pp., Registrované v: WOS

ADCA215 KUBOTA, Yoshiyuki - OHNUMA, Toshiharu - BUČKO, Tomáš. Carbon dioxide capture in 2-aminoethanol aqueous solution from ab initio molecular dynamics simulations. In *Journal of Chemical Physics*, 2016, vol. 146, no. 9, 094303-1-094303-9. (2015: 2.894 - IF, Q2 - JCR, 0.953 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] SEVGEN, Emre - GIBERTI, Federico - SIDKY, Hythem - WHITMER, Jonathan K. - GALLI, Giulia - GYGI, Francois - DE PABLO, Juan J. Hierarchical Coupling of First-Principles Molecular Dynamics with Advanced Sampling Methods. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 6, pp. 2881-2888., Registrované v: WOS

ADCA216 KÚDELA, Stanislav - GERGELY, Vladimír - SMRČOK, Ľubomír - OSWALD, Steffen - BAUNACK, Stefan - WETZIG, Klaus. Phase transformations of delta Al₂O₃ (Saffil) fibres during their interaction with molten MgLi alloys.

Citácie:

1. [1.1] LIU, Ningning - WU, Yunhai - SHA, Haitao. Characterization of EDTA-cross-linked beta-cyclodextrin grafted onto Fe-Al hydroxides as an efficient adsorbent for methylene blue. In *JOURNAL OF COLLOID AND INTERFACE SCIENCE*. ISSN 0021-9797, 2018, vol. 516, no., pp. 98-109., Registrované v: WOS

ADCA217 KUCHARÍK, Marián - BOČA, Miroslav - BESSADA, Catherine - FUESS, H. Do sodium oxofluoroaluminates exist at room temperature? In *European Journal of Inorganic Chemistry*, 2005, no. 9, p. 1781-1786. ISSN 1434-1948.

Citácie:

1. [1.1] KONTRIK, Martin - SIMKO, Frantisek - GALUSKOVA, Dagmar - NOSKO, Martin - BIZOVSKA, Valeria - HICAK, Michal - GALUSEK, Dusan - RAKHMATULLIN, Aydar - KORENKO, Michal. A corrosion mechanism of titanium diboride in KF AlF₃ Al₂O₃ melt. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 4, pp. 1143-1151., Registrované v: WOS

- ADCA218 BIZOVSKÁ, Valéria - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana. Montmorillonite modified with unconventional surfactants from the series of octylammonium-based cations: Structural characterization and hydration properties. In *Applied Clay Science*, 2018, vol. 158, p. 102-112. (2017: 3.641 - IF, Q1 - JCR, 0.992 - SJR, Q1 - SJR, karentované - CCC). (2018 - Current Contents). ISSN 0169-1317.
- Citácie:
1. [1.1] *SUN, Baohong - ZHANG, Ming - ZHOU, Ninglin - CHU, Xiaohong - YUAN, Ping - CHI, Cheng - WU, Fan - SHEN, Jian. Study on montmorillonite-chlorhexidine acetate-terbinafine hydrochloride intercalation composites as drug release systems. In RSC ADVANCES. ISSN 2046-2069, 2018, vol. 8, no. 38, pp. 21369-21377., Registrované v: WOS*
- ADCA219 BIZOVSKÁ, Valéria - PÁLKOVÁ, Helena - MADEJOVÁ, Jana. Near-infrared study of water adsorption on homo-ionic forms of montmorillonite. In *Clays and Clay Minerals*, 2016, vol. 64, no. 5, p. 571-585. (2015: 1.222 - IF, Q3 - JCR, 0.504 - SJR, Q2 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0009-8604.
- Citácie:
1. [1.1] *TSIANTOS, C. - GIONIS, V. - CHRYSIKOS, G. D. Smectite in bentonite: Near infrared systematics and estimation of layer charge. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 160, no., pp. 81-87., Registrované v: WOS*
- ADCA220 LANGER, Vratislav - SMRČOK, Ľubomír - BOČA, Miroslav. Redetermination of Na₃TaF₈. In *Acta Crystallographica Section C. Crystal Structure Communications*, 2010, vol. 66, p. 85-86. (2009: 0.782 - IF, karentované - CCC). (2010 - Current Contents). ISSN 0108-2701.
- Citácie:
1. [1.1] *DENG, T. T. - SONG, E. H. - SU, J. - ZHOU, Y. Y. - WANG, L. Y. - YE, S. - ZHANG, Q. Y. Stable narrowband red emission in fluorotellurate KTeF₅:Mn⁴⁺ via Mn⁴⁺ noncentral-site occupation. In JOURNAL OF MATERIALS CHEMISTRY C. ISSN 2050-7526, 2018, vol. 6, no. 16, pp. 4418-4426., Registrované v: WOS*
- ADCA221 LANGER, Vratislav - SCHOLTZOVÁ, Eva - GYEPESOVÁ, Dalma - KOHÚTOVÁ, Mária - VALENT, A. (1-Methylimidazole)(N-salicylidene-rac-glutamato) copper(II). In *Acta Crystallographica Section E*, 2003, vol. 59, p. m1181-m1183. ISSN 1600-5368.
- Citácie:
1. [1.1] *MUCHE, Simon - HARMS, Klaus - BURGHHAUS, Olaf - HOLYNSKA, Malgorzata. A gap is filled: First structures of enantiopure iron(III) complexes with Schiff base ligands derived from ortho-vanillin and L-glutamine or L-glutamic acid. In POLYHEDRON. ISSN 0277-5387, 2018, vol. 144, no., pp. 66-74., Registrované v: WOS*
- ADCA222 LANGER, Vratislav - SCHOLTZOVÁ, Eva - GYEPESOVÁ, Dalma - KOHÚTOVÁ, Mária - VALENT, A. (N-salicylidene-D,L-glutamato)(2-methylimidazole)copper(II). In *Acta Crystallographica E*, 2004, vol. 60, p. M129-M132. ISSN 1600-5368.
- Citácie:
1. [1.1] *MUCHE, Simon - HARMS, Klaus - BURGHHAUS, Olaf - HOLYNSKA, Malgorzata. A gap is filled: First structures of enantiopure iron(III) complexes with Schiff base ligands derived from ortho-vanillin and L-glutamine or L-glutamic acid. In POLYHEDRON. ISSN 0277-5387, 2018, vol. 144, no., pp. 66-74., Registrované v: WOS*
- ADCA223 LANGER, Vratislav - GYEPESOVÁ, Dalma - MACH, Pavel - SCHOLTZOVÁ, Eva - SALIŠOVÁ, M. - BOHÁČ, A. - GAŠPÁR, B. anti-2-hydroxy-2-methyl-1-tetralone oxime: X-ray and density functional theory study. In *Acta Crystallographica C*, 2006, vol. 62, p. o199-o202.
- Citácie:
1. [1.1] *OWSIANIK, Krzysztof - KRAWCZYK, Ewa - MIELNICZAK, Grazyna - KOPROWSKI, Marek - SIERON, Leslaw. Three-step synthesis of chiral and sterically hindered amino alcohols based on cyclic enol phosphates. In TETRAHEDRON. ISSN 0040-4020, 2018, vol. 74, no. 51, pp. 7343-7350., Registrované v: WOS*
- ADCA224 LANG, Jakub - ŠVAŇA, Matej - DEMEL, Ondřej - BRABEC, Jiří - KEDŽUCH, Stanislav - NOGA, Jozef - KOWALSKI, Karol - PITTNER, Jiří. A MRCC study of the isomerisation of cyclopropane. In *Molecular Physics*, 2017, vol. 115, no. 21-22, p. 2743-2754. (2016: 1.870 - IF, Q2 - JCR, 0.820 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0026-8976.
- Citácie:
1. [1.1] *COUGHTRIE, David J. - GIERETH, Robin - KATS, Daniel - WERNER, Hans Joachim - KOEHN, Andreas. Embedded Multireference Coupled Cluster Theory. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 2, pp. 693-709., Registrované v: WOS*
- ADCA225 LAZAR, Petr - BUČKO, Tomáš - HAFNER, Jürgen. Negative thermal expansion of ScF₃: Insights from density-functional molecular dynamics in the isothermal-isobaric ensemble. In *Physical Review B*, 2015, vol. 92, no. 22, p. 224302-1-224302. (2014: 3.736 - IF, Q1 - JCR, 2.656 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents, WOS, SCOPUS). ISSN 1550-235X.
- Citácie:
1. [1.1] *GUPTA, M. K. - SINGH, Baltej - MITTAL, R. - CHAPLOT, S. L. Negative thermal expansion behavior in MZrF₆ (M = Ca, Mg, Sr): Ab initio lattice dynamical studies. In PHYSICAL REVIEW B. ISSN 2469-9950, 2018, vol. 98, no. 1, pp., Registrované v: WOS*
2. [1.1] *MITTAL, R. - GUPTA, M. K. - CHAPLOT, S. L. Phonons and anomalous thermal expansion behaviour in crystalline solids. In PROGRESS IN MATERIALS SCIENCE. ISSN 0079-6425, 2018, vol. 92, no., pp. 360-445., Registrované v: WOS*
3. [1.1] *SINGH, Baltej - GUPTA, Mayanak K. - MITTAL, Ranjan - CHAPLOT, Samrath L. Density Functional Studies Revealing Anomalous Lattice Behavior in Metal Cyanide, AgC₈N₅. In JOURNAL OF PHYSICAL CHEMISTRY C. ISSN 1932-7447, 2018, vol. 122, no. 27, pp. 15575-15581., Registrované v: WOS*
4. [1.1] *SINGH, Baltej - GUPTA, Mayanak K. - MITTAL, Ranjan - ZBIRI, Mohamed - HODGSON, Sarah A. - GOODWIN, Andrew*

L. - SCHÖBER, Helmut - CHAPLOT, Samrath L. Anomalous Lattice Dynamics in AgC₄N₃: Insights From Inelastic Neutron Scattering and Density Functional Calculations. In *FRONTIERS IN CHEMISTRY*. ISSN 2296-2646, 2018, vol. 6, no., pp., Registrované v: WOS

5. [1.1] WINTER, I. S. - MONTROYA, J. - PERSSON, K. A. - CHRZAN, D. C. Ab initio calculation of thermal expansion with application to understanding Invar behavior in gum metal. In *PHYSICAL REVIEW MATERIALS*. ISSN 2475-9953, 2018, vol. 2, no. 7, pp., Registrované v: WOS

ADCA226 LENČEŠ, Zoltán - PENTRÁKOVÁ, Linda - HRABALOVÁ, Monika - ŠAJGALÍK, Pavol - HIRAO, Kiyoshi. Decomposition of MgSiN₂ in nitrogen atmosphere. In *Journal of the European Ceramic Society*, 2011, vol. 31, no. 8, p. 1473-1480. (2010: 2.574 - IF, karentované - CCC). (2011 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] KAEWMEECHAI, Chaiyawat - LAOSIRITAWORN, Yongyut - JAROENJITTICHA, Atchara Punya. First-principles calculations of zone center phonons and related thermal properties of MgSiN₂. In *SIAM PHYSICS CONGRESS 2017 (SPC2017)*. ISSN 1742-6588, 2017, vol. 901, no., pp., Registrované v: WOS

ADCA227 LENČEŠ, Zoltán - HIRAO, Kiyoshi - YAMAUCHI, Yukihiro - KANZAKI, Shuzo. Reaction synthesis of magnesium silicon nitride powder. In *Journal of the American Ceramic Society*, 2003, vol. 86, no. 7, p. 1088-1093. (2002: 1.796 - IF, karentované - CCC). (2003 - Current Contents). ISSN 0002-7820.

Citácie:

1. [1.1] HAEUSLER, Jonas - NIKLAUS, Robin - MINAR, Jan - SCHNICK, Wolfgang. Ammonothermal Synthesis and Optical Properties of Ternary Nitride Semiconductors Mg-IV-N-2, Mn-IV-N-2 and Li-IV-N-3 (IV=Si, Ge). In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 7, pp. 1686-1693., Registrované v: WOS

2. [1.1] REIN, Viktor - WENZEL, Olivia - POPESCU, Radian - GERTHSEN, Dagmar - FELDMANN, Claus. Liquid-ammonia synthesis of microporous Mg₃N₂ showing intense red-light emission. In *JOURNAL OF MATERIALS CHEMISTRY C*. ISSN 2050-7526, 2018, vol. 6, no. 16, pp. 4450-4456., Registrované v: WOS

3. [1.1] ZHANG, Kailong - LU, Juanjuan - ZHAO, Dejian - WANG, Liangbiao - QIN, Hengfei - LIU, Weiqiao - MEI, Tao. Sulfur-assisted Synthesis of Magnesium Silicon Nitride Nanoparticles at Low Temperature. In *CHEMISTRY LETTERS*. ISSN 0366-7022, 2018, vol. 47, no. 10, pp. 1318-1320., Registrované v: WOS

ADCA228 LICHVÁR, Peter - LIŠKA, Marek - GALUSEK, Dušan. What is the true Kramers-Kronig transform? In *Ceramics - Silikáty*. - Praha : Institut of Chemical Technology : Institute of Inorganic Chemistry (Academy of Sciences ČR), 2002, vol. 46, no. 1, p. 25-27. (2001: 0.167 - IF). ISSN 0862-5468.

Citácie:

1. [1.1] MAYERHOEFER, Thomas G. - PAHLOW, Susanne - HUEBNER, Uwe - POPP, Juergen. Removing interference-based effects from the infrared transmittance spectra of thin films on metallic substrates: a fast and wave optics conform solution. In *ANALYST*. ISSN 0003-2654, 2018, vol. 143, no. 13, pp. 3164-3175., Registrované v: WOS

ADCA229 LINCK, Christoph - IONESCU, Emanuel - PAPENDORF, Benjamin - GALUSKOVÁ, Dagmar - GALUSEK, Dušan - ŠAJGALÍK, Pavol - RIEDEL, Ralf. Corrosion behavior of silicon oxycarbide-based ceramic nanocomposites under hydrothermal conditions. In *International Journal of Materials Research*, 2012, vol. 103, no. 1, p. 31-39. (2011: 0.830 - IF, 0.573 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 1862-5282.

Citácie:

1. [1.1] BRINCKMANN, Stephan A. - PATRA, Niranjana - YAO, Jia - WARE, Taylor H. - FRICK, Carl P. - FERTIG, Ray S. Stereolithography of SiOC Polymer-Derived Ceramics Filled with SiC Micronwhiskers. In *ADVANCED ENGINEERING MATERIALS*. ISSN 1438-1656, 2018, vol. 20, no. 11, pp., Registrované v: WOS

2. [1.1] LU, Kathy - ERB, Donald. Polymer derived silicon oxycarbide-based coatings. In *INTERNATIONAL MATERIALS REVIEWS*. ISSN 0950-6608, 2018, vol. 63, no. 3, pp. 139-161., Registrované v: WOS

3. [1.1] ROBLES, Eduardo - CSOKA, Levente - LABIDI, Jalel. Effect of Reaction Conditions on the Surface Modification of Cellulose Nanofibrils with Aminopropyl Triethoxysilane. In *COATINGS*. ISSN 2079-6412, 2018, vol. 8, no. 4, pp., Registrované v: WOS

ADCA230 LIN, Su-Shia - HUANG, J.-L. - ŠAJGALÍK, Pavol. The properties of Ti-doped ZnO films deposited by simultaneous RF and DC magnetron sputtering. In *Surface and coatings technology*, 2005, vol. 191, no. 2-3, p. 286-292. ISSN 0257-8972.

Citácie:

1. [1.1] ISAWI, Heba. Development of thin-film composite membranes via radical grafting with methacrylic acid/ZnO doped TiO₂ nanocomposites. In *REACTIVE & FUNCTIONAL POLYMERS*. ISSN 1381-5148, 2018, vol. 131, no., pp. 400-413., Registrované v: WOS

2. [1.1] LI, Bao-Jia - WANG, Yong-Ying - HUANG, Li-Jing - CAO, Hai-Di - WANG, Qinghua - REN, Nai-Fei - DING, Hongtao. Ultrasonic-vibration-assisted laser annealing of fluorine-doped tin oxide thin films for improving optical and electrical properties: Overlapping rate. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 18, pp. 22225-22234., Registrované v: WOS

3. [1.1] LIU, Wei-Sheng - HSIEH, Wei-Ting - CHEN, Shih-Yuan - HUANG, Chien-Sheng. Improvement of CIGS solar cells with high performance transparent conducting Ti-doped GaZnO thin films. In *SOLAR ENERGY*. ISSN 0038-092X, 2018, vol. 174, no., pp. 83-96., Registrované v: WOS

4. [1.1] MUNIR, T. - KASHIF, M. - HUSSAIN, W. - SHAHZAD, A. - IMRAN, M. - AHMED, A. - AMIN, N. - AHMED, N. - HUSSAIN, A. - NOREEN, M. FIRST PRINCIPLES STUDY OF STRUCTURAL AND ELECTRONIC PROPERTIES OF Ti DOPED ZnO. In *JOURNAL OF OVONIC RESEARCH*. ISSN 1842-2403, 2018, vol. 14, no. 5, pp. 333-337., Registrované v: WOS

5. [1.1] NURFANI, Eka - SATRYA, Christoforus Dimas - ABDURRAHMAN, Irfan - SUTJAHJA, Inge Magdalena - WINATA, Toto - TAKASE, Kouichi - RUSYDI, Andriyo - DARMA, Yudi. Weakening of excitonic screening effects in Ti_xZn_{1-x}O thin films. In *THIN*

- SOLID FILMS. ISSN 0040-6090, 2018, vol. 645, no., pp. 399-404., Registrované v: WOS*
6. [1.1] SUN, Wenming - ZHANG, Liang - ZHANG, Yanpeng - LIU, Jing - WANG, Hong - BU, Yuxiang. Enhanced works of separation for (0001) ZnO vertical bar(111) ZnO2 interfaces via ion-doping in ZnO: Data-mining and density function theory study. In *COMPUTATIONAL MATERIALS SCIENCE. ISSN 0927-0256, 2018, vol. 142, no., pp. 410-416., Registrované v: WOS*
- ADCA231 LIN, Su-Shia - HUANG, J.-L. - ŠAJGALÍK, Pavol. Effects of substrate temperature on the properties of heavily Al-doped ZnO films by simultaneous r.f. and d.c. magnetron sputtering. In *Surface and coatings technology, 2005, vol. 190, no. 1, p. 39-47. ISSN 0257-8972.*
- Citácie:
1. [1.1] SRIPIANEM, Worapot - TECHAPIESANCHAROENKIJ, Ratchatee. Effect of Al and Ga codoping on the morphological, electronic, and optical properties of ZnO transparent conductive thin films prepared by spray pyrolysis technique. In *TURKISH JOURNAL OF PHYSICS. ISSN 1300-0101, 2018, vol. 42, no. 6, pp. 688-698., Registrované v: WOS*
- ADCA232 LIN, Su-Shia - HUANG, J.-L. - ŠAJGALÍK, Pavol. The properties of heavily Al-doped ZnO films before and after annealing in the different atmosphere. In *Surface and coatings technology, 2004, vol. 185, no. 2-3, p. 254-263. ISSN 0257-8972.*
- Citácie:
1. [1.1] BISHNOI, Swati - RAJESH, B. - SWATI, G. - JAISWAL, Vishnu Vikesh - SAHU, Mukesh - SINGH, Paramjeet - HARANATH, D. Structural, morphological, photoluminescence and electrical characterization of aluminium doped ZnO phosphors for solar cell applications. In *MATERIALS TODAY-PROCEEDINGS. ISSN 2214-7853, 2018, vol. 5, no. 1, pp. 610-619., Registrované v: WOS*
- ADCA233 LIŠKA, Marek - PERICHTA, P. - TURI NAGY, L.. The structure of MD simulated cryolite melt. In *Journal of Non-Crystalline Solids, 1995, vol. 192-193, p. 309-311. (1994: 1.070 - IF, karentované - CCC). (1995 - Current Contents). ISSN 0022-3093.*
- Citácie:
1. [1.1] BUCKO, Tomas - SIMKO, Frantisek. Effect of alkaline metal cations on the ionic structure of cryolite melts: Ab-initio NpT MD study. In *JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 6, pp., Registrované v: WOS*
- ADCA234 LIŠKA, Marek - ŠIMURKA, Peter - ANTALÍK, J. - PERICHTA, P. Viscosity of titania-bearing sodium silicate melts. In *Chemical Geology, 1996, vol. 128, no. 1-4, p. 199-206. ISSN 0009-2541.*
- Citácie:
1. [1.1] CUI, Shaogang - ZHU, Hongtao - WAN, Shanrong - BACH TRAN - WANG, Long - TIEU, Kiet. Investigation of different inorganic chemical compounds as hot metal forming lubricant by pin-on-disc and hot rolling. In *TRIBOLOGY INTERNATIONAL. ISSN 0301-679X, 2018, vol. 125, no., pp. 110-120., Registrované v: WOS*
- ADCA235 LOFAJ, Marcel - VALENT, Ivan - BUJDÁK, Juraj. Mechanism of rhodamine 6G molecular aggregation in montmorillonite colloid. In *Central European Journal of Chemistry, 2013, vol. 11, no. 10, p. 1606-1619. (2012: 1.167 - IF, 0.372 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 1895-1066.(APVV-0291-11 : Fotoaktívne hybridné nanomateriály s luminiscenčnými a antimikrobiálnymi vlastnosťami).*
- Citácie:
1. [1.1] CHAPMAN, Mingyu - EULER, William B. Rhodamine 6G Structural Changes in Water/Ethanol Mixed Solvent. In *JOURNAL OF FLUORESCENCE. ISSN 1053-0509, 2018, vol. 28, no. 6, pp. 1431-1437., Registrované v: WOS*
2. [1.1] KOCHERVINSKII, V. V. - KOZLOVA, N. V. - SHMAKOVA, N. A. - KALABUKHOVA, A. V. - KISELEV, D. A. - MALINKOVICH, M. D. - GRADOVA, M. A. - GRADOV, O. V. - BEDIN, S. A. Influence of Dye Molecules on the Polarization of Ferroelectric Vinylidene Fluoride Copolymer. In *CRYSTALLOGRAPHY REPORTS. ISSN 1063-7745, 2018, vol. 63, no. 6, pp. 983-988., Registrované v: WOS*
- ADCA236 MACA, Karel - POUCHLÝ, Václav - BODIŠOVÁ, Katarína - ŠVANČÁREK, Peter - GALUSEK, Dušan. Densification of fine-grained alumina ceramics doped by magnesia, yttria and zirconia evaluated by two different sintering models. In *Journal of the European Ceramic Society, 2014, vol. 34, no. 16, p. 4363-4372. (2013: 2.307 - IF, 1.122 - SJR, karentované - CCC). (2014 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.*
- Citácie:
1. [1.1] EL-MEHALAWY, N. - AWAAD, M. - ELIYAN, T. - ABD-ALLAH, M. A. - NAGA, S. M. Electrical properties of ZnO/alumina nano composites for high voltage transmission line insulator. In *JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS. ISSN 0957-4522, 2018, vol. 29, no. 16, pp. 13526-13533., Registrované v: WOS*
2. [1.1] FRUEH, T. - OZER, I. O. - POTERALA, S. F. - LEE, H. - KUPP, E. R. - COMPSON, C. - ATRIA, J. - MESSING, G. L. A critique of master sintering curve analysis. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY. ISSN 0955-2219, 2018, vol. 38, no. 4, pp. 1030-1037., Registrované v: WOS*
3. [1.1] YU, Hui - XU, Zhihao - WEI, Ziye - CHEN, Yongjun - LI, Jianbao - LUO, Lijie. Effect of talc and titania on the microstructure and mechanical properties of alumina ceramics. In *INTERNATIONAL JOURNAL OF APPLIED CERAMIC TECHNOLOGY. ISSN 1546-542X, 2018, vol. 15, no. 3, pp. 633-642., Registrované v: WOS*
- ADCA237 MADEJOVÁ, Jana - PENTRÁK, Martin - PÁLKOVÁ, Helena - KOMADEL, Peter. Near-infrared spectroscopy: A powerful tool in studies of acid-treated clay minerals. In *Vibrational Spectroscopy, 2009, vol. 49, no. 2, p. 211-218. (2008: 1.810 - IF, karentované - CCC). (2009 - Current Contents). ISSN 0924-2031.*
- Citácie:
1. [1.1] CHEN, Shuling - HONG, Hanlie - HUANG, Xianyu - FANG, Qian - YIN, Ke - WANG, Chaowen - ZHANG, Yiming - CHENG, Liuling - ALGEO, Thomas J. The role of organo-clay associations in limiting organic matter decay: Insights from the Dajiuhe peat soil, central China. In *GEODERMA. ISSN 0016-7061, 2018, vol. 320, no., pp. 149-160., Registrované v: WOS*

2. [1.1] CUEVAS, Jaime - ISABEL RUIZ, Ana - FERNANDEZ, Raul. Investigating the Potential Barrier Function of Nanostructured Materials Formed in Engineered Barrier Systems (EBS) Designed for Nuclear Waste Isolation. In *CHEMICAL RECORD*. ISSN 1527-8999, 2018, vol. 18, no. 7-8, pp. 1065-1075., Registrované v: WOS
 3. [1.1] FUKS, L. - HERDZIK-KONIECKO, I. Vermiculite as a potential component of the engineered barriers in low- and medium-level radioactive waste repositories. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 161, no., pp. 139-150., Registrované v: WOS
 4. [1.1] LI, Zijong - GUO, Jilong - DONG, Zhao - CHEN, Jiawei. Insight into interactions of olivine-scCO₂-water system at 140 degrees C and 15 MPa during CO₂ mineral sequestration. In *GEOSCIENCE FRONTIERS*. ISSN 1674-9871, 2018, vol. 9, no. 6, pp. 1945-1955., Registrované v: WOS
 5. [1.1] PASSOS, Elthon Ferreira - MARANGONI, Rafael - ZATTA, Leandro. Cassava Starch-Based Films Reinforced with Clay Minerals. In *ORBITAL-THE ELECTRONIC JOURNAL OF CHEMISTRY*. ISSN 1984-6428, 2018, vol. 10, no. 7, pp. 523-534., Registrované v: WOS
 6. [1.1] RITZ, Michal - VALASKOVA, Marta. Infrared and Raman spectroscopy of three commercial vermiculites doped with cerium dioxide nanoparticles. In *SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY*. ISSN 1386-1425, 2018, vol. 201, no., pp. 39-45., Registrované v: WOS
- ADCA238 MADEJOVÁ, Jana - KOMADEL, Peter - ČÍČEL, Blahoslav. Infrared study of octahedral site populations in smectites. In *Clay Minerals*, 1994, vol. 29, no. 3, p. 319-326. ISSN 0009-8558.
- Citácie:
1. [1.1] CERVINI-SILVA, Javiera - PALACIOS, Eduardo - GOMEZ-VIDALES, Virginia. Nontronite as natural source and growth template for (nano)maghemite [γ -Fe₂O₃] and (nano)Wustite [Fe_{1-x}O]. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 156, no., pp. 178-186., Registrované v: WOS
 2. [1.1] PELAYO, M. - MARCO, J. F. - FERNANDEZ, A. M. - VERGARA, L. - MELON, A. M. - PEREZ DEL VILLAR, L. Infrared and Mossbauer spectroscopy of Fe-rich smectites from Morron de Mateo bentonite deposit (Spain). In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 1, pp. 17-28., Registrované v: WOS
- ADCA239 MADEJOVÁ, Jana - BUJDÁK, Juraj - GATES, W.P. - KOMADEL, Peter. Preparation and infrared spectroscopic characterization of reduced-charge montmorillonite with various Li contents. In *Clay Minerals*, 1996, vol. 31, no. 2, p. 233-241. ISSN 0009-8558.
- Citácie:
1. [1.1] DAMIAN, Gheorghe - LANZERSTORFER, Christof - DAMIAN, Floarea - IEPURE, Gheorghe. Distribution of Heavy Metals and Minerals in the Various Size Fractions of Soil from CopE (TM) a Mic, RomAnia. In *WATER AIR AND SOIL POLLUTION*. ISSN 0049-6979, 2018, vol. 229, no. 6, pp., Registrované v: WOS
 2. [1.1] PALCHIK, N. A. - MOROZ, T. N. - MIROSHNICHENKO, L. V. Structure and Properties of Syntetic Layered Lithium-Containing Silicates. In *CRYSTALLOGRAPHY REPORTS*. ISSN 1063-7745, 2018, vol. 63, no. 7, pp. 1082-1087., Registrované v: WOS
 3. [1.1] QIANG, Tang - FAN, Gu - GAO YUFENG - TORU, Inui - TAKESHI, Katsumi. Desorption characteristics of Cr(III), Mn(II), and Ni(II) in contaminated soil using citric acid and citric acid-containing wastewater. In *SOILS AND FOUNDATIONS*. ISSN 0038-0806, 2018, vol. 58, no. 1, pp. 50-64., Registrované v: WOS
 4. [1.1] SCHIEBEL, Korbinian - JORDAN, Guntram - KAESTNER, Anders - SCHILLINGER, Burkhard - GEORGII, Robert - HESS, Kai-Uwe - BOEHNKE, Sandra - SCHMAHL, Wolfgang W. Effects of heat and cyclic reuse on the properties of bentonite-bonded sand. In *EUROPEAN JOURNAL OF MINERALOGY*. ISSN 0935-1221, 2018, vol. 30, no. 6, pp. 1115-1125., Registrované v: WOS
- ADCA240 MADEJOVÁ, Jana - BUJDÁK, Juraj - JANEK, Marián - KOMADEL, Peter. Comparative FT-IR study of structural modifications during acid treatment of dioctahedral smectites and hectorite. In *Spectrochimica Acta Part A - Molecular and Biomolecular Spectroscopy*, 1988, vol. 54, no. 10, p. 1397-1406. ISSN 1386-1425.
- Citácie:
1. [1.1] ANTONIO CECILIA, Juan - PARDO, Laura - POZO, Manuel - BELLIDO, Eva - FRANCO, Francisco. Microwave-Assisted Acid Activation of Clays Composed of 2:1 Clay Minerals: A Comparative Study. In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 9, pp., Registrované v: WOS
 2. [1.1] BELHOCINE, M. - HAOUZI, A. - BASSOU, G. - PHOU, T. - MAURIN, D. - BANTIGNIES, J. L. - HENN, F. Isothermic heat of water adsorption and desorption in homoionic alkaline-earth montmorillonites. In *CHEMICAL PHYSICS*. ISSN 0301-0104, 2018, vol. 501, no., pp. 26-34., Registrované v: WOS
 3. [1.1] BRITO, Deoclecio F. - DA SILVA FILHO, Edson C. - FONSECA, Maria G. - JABER, Maguy. Organophilic bentonites obtained by microwave heating as adsorbents for anionic dyes. In *JOURNAL OF ENVIRONMENTAL CHEMICAL ENGINEERING*. ISSN 2213-2929, 2018, vol. 6, no. 6, pp. 7080-7090., Registrované v: WOS
 4. [1.1] CHAVALI, Rama Vara Prasad - REDDY, Hari Prasad P. VOLUME CHANGE BEHAVIOR OF PHOSPHOGYPSUM TREATED CLAYEY SOILS CONTAMINATED WITH INORGANIC ACIDS A MICRO LEVEL STUDY. In *JOURNAL OF ENVIRONMENTAL ENGINEERING AND LANDSCAPE MANAGEMENT*. ISSN 1648-6897, 2018, vol. 26, no. 1, pp. 8-18., Registrované v: WOS
 5. [1.1] DOS SANTOS, E. C. - GATES, W. P. - MICHELS, L. - JURANYI, F. - MIKKELSEN, A. - DA SILVA, G. J. - FOSSUM, J. O. - BORDALLO, H. N. The pH influence on the intercalation of the bioactive agent ciprofloxacin in fluorohectorite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 166, no., pp. 288-298., Registrované v: WOS
 6. [1.1] DUTTA, Dipak Kumar. Clay mineral catalysts. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS*, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 289-329., Registrované v: WOS
 7. [1.1] HAI, Chunxi - ZHOU, Yuan - FUJI, Masayoshi - SHIRAI, Takashi - REN, Xiufeng - ZENG, Jinbo - LI, Xiang. Electrical conductivity of hydrothermally synthesized sodium lithium magnesium silicate. In *MATERIALS RESEARCH BULLETIN*. ISSN 0025-5408, 2018, vol. 97, no., pp. 473-482., Registrované v: WOS
 8. [1.1] JIAN, Xingwen - HUANG, Jing - CAI, Zhenlei - ZHANG, Yimin - LIU, Tao - LIU, Hong. Effect of alkaline fusion on

muscovite decomposition and the vanadium release mechanism from vanadium shale. In ROYAL SOCIETY OPEN SCIENCE. ISSN 2054-5703, 2018, vol. 5, no. 10, pp., Registrované v: WOS

9. [1.1] MARCO CHAMBI-PERALTA, Marvin - VIEIRA COELHO, Antonio Carlos - DE SOUZA CARVALHO, Flavio Machado - TOFFOLI, Samuel Marcio. Effects of exchanged cation, acid treatment and high shear mechanical treatment on the swelling and the particle size distribution of vermiculite. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 155, no., pp. 1-7., Registrované v: WOS

10. [1.1] NAKHLI, Asma - MBOUGA, Marie Goletti Ngumtchouin - BERGAOUI, Manel - KHALFAOUI, Mohamed - CRETIN, Marc - HUGUET, Patrice. Modeling of essential oils adsorption onto clays towards a better understanding of their interactions. In JOURNAL OF MOLECULAR LIQUIDS. ISSN 0167-7322, 2018, vol. 249, no., pp. 132-143., Registrované v: WOS

11. [1.1] RITZ, Michal - VALASKOVA, Marta. Infrared and Raman spectroscopy of three commercial vermiculites doped with cerium dioxide nanoparticles. In SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY. ISSN 1386-1425, 2018, vol. 201, no., pp. 39-45., Registrované v: WOS

12. [1.1] ROCHA, Mariana - COSTA, Paula - SOUSA, Carlos A. D. - PEREIRA, Clara - RODRIGUEZ-BORGES, Jose E. - FREIRE, Cristina. L-serine-functionalized montmorillonite decorated with Au nanoparticles: A new highly efficient catalyst for the reduction of 4-nitrophenol. In JOURNAL OF CATALYSIS. ISSN 0021-9517, 2018, vol. 361, no., pp. 143-155., Registrované v: WOS

13. [1.1] TERZIC, Anja - PEZO, Lato - MIJATOVIC, Nevenka - STOJANOVIC, Jovica - KRAGOVIC, Milan - MILICIC, Ljiljana - ANDRIC, Ljubisa. The effect of alternations in mineral additives (zeolite, bentonite, fly ash) on physico-chemical behavior of Portland cement based binders. In CONSTRUCTION AND BUILDING MATERIALS. ISSN 0950-0618, 2018, vol. 180, no., pp. 199-210., Registrované v: WOS

14. [1.1] WEGRZYN, Agnieszka - STAWINSKI, Wojciech - FREITAS, Olga - KOMEDERA, Kamila - BLACHOWSKI, Artur - JECZMIONEK, Lukasz - DANKO, Tomasz - MORDARSKI, Grzegorz - FIGUEIREDO, Sonia. Study of adsorptive materials obtained by wet fine milling and acid activation of vermiculite. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 155, no., pp. 37-49., Registrované v: WOS

15. [1.1] ZAHAF, Faiza - MAROUF, Reda - OUADJENIA, Fatima - SCHOTT, Jacques. Kinetic and thermodynamic studies of the adsorption of Pb(II), Cr(III) and Cu(II) onto modified bentonite. In DESALINATION AND WATER TREATMENT. ISSN 1944-3994, 2018, vol. 131, no., pp. 282-290., Registrované v: WOS

16. [1.1] ZHAO, Longsheng - WANG, Lina - QI, Tao - CHEN, Desheng - ZHAO, Hongxin - LIU, Yahui - WANG, Weijing. Leaching of Titanium and Silicon from Low-Grade Titanium Slag Using Hydrochloric Acid Leaching. In JOM. ISSN 1047-4838, 2018, vol. 70, no. 10, pp. 1985-1990., Registrované v: WOS

ADCA241 MADEJOVÁ, Jana - PÁLKOVÁ, Helena - KOMADEL, Peter. Behaviour of Li⁺ and Cu²⁺ in heated montmorillonite: Evidence from far-, mid-, and near-IR regions. In Vibrational Spectroscopy, 2006, vol. 40, no. 1, p. 80-88. ISSN 0924-2031.

Citácie:

1. [1.1] BODART, Philippe R. - DELMOTTE, L. - RIGOLET, S. - BRENDLE, J. - GOUGEON, Regis D. Li-7{F-19} TEDOR NMR to observe the lithium migration in heated montmorillonite. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 157, no., pp. 204-211., Registrované v: WOS

ADCA242 MADEJOVÁ, Jana - PÁLKOVÁ, Helena - JANKOVIČ, Ľuboš. Near-infrared study of the interaction of pyridine with acid-treated montmorillonite. In Vibrational Spectroscopy, 2015, vol. 76, p. 22-30. (2014: 2.003 - IF, Q2 - JCR, 0.522 - SJR, Q3 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0924-2031.

Citácie:

1. [1.1] BOUCLY, Anthony - ROCHET, Francois - ARNOUX, Quentin - GALLET, Jean-Jacques - BOURNEL, Fabrice - TISSOT, Heloise - MARRY, Virginie - DUBOIS, Emmanuelle - MICHOT, Laurent. Soft X-ray Heterogeneous Radiolysis of Pyridine in the Presence of Hydrated Strontium-Hydroxyhectorite and its Monitoring by Near-Ambient Pressure Photoelectron Spectroscopy. In SCIENTIFIC REPORTS. ISSN 2045-2322, 2018, vol. 8, no., pp., Registrované v: WOS

2. [1.1] VELTHOEN, Marjolein E. Z. - MUNOZ-MURILLO, Ara - BOUHMADI, Abdelkbir - CECIUS, Michael - DIEFENBACH, Steve - WECKHUYSEN, Bert M. The Multifaceted Role of Methylaluminoxane in Metallocene-Based Olefin Polymerization Catalysis. In MACROMOLECULES. ISSN 0024-9297, 2018, vol. 51, no. 2, pp. 343-355., Registrované v: WOS

ADCA243 MADEJOVÁ, Jana - BUJDÁK, Juraj - PETIT, Sabine - KOMADEL, Peter. Effects of chemical composition and temperature of heating on the infrared spectra of Li-saturated dioctahedral smectites. (I) Mid-infrared region. In Clay Minerals, 2000, vol. 35, no 5, p. 739-751. (1999: 1.090 - IF). ISSN 0009-8558.

Citácie:

1. [1.1] BODART, Philippe R. - DELMOTTE, L. - RIGOLET, S. - BRENDLE, J. - GOUGEON, Regis D. Li-7{F-19} TEDOR NMR to observe the lithium migration in heated montmorillonite. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 157, no., pp. 204-211., Registrované v: WOS

2. [1.1] PELAYO, M. - MARCO, J. F. - FERNANDEZ, A. M. - VERGARA, L. - MELON, A. M. - PEREZ DEL VILLAR, L. Infrared and Mossbauer spectroscopy of Fe-rich smectites from Morron de Mateo bentonite deposit (Spain). In CLAY MINERALS. ISSN 0009-8558, 2018, vol. 53, no. 1, pp. 17-28., Registrované v: WOS

ADCA244 MADEJOVÁ, Jana - BUJDÁK, Juraj - PETIT, Sabine - KOMADEL, Peter. Effects of chemical composition and temperature of heating on the infrared spectra of Li-saturated dioctahedral smectites. (II) Near-infrared region. In Clay Minerals, 2000, vol. 35, no. 5, p. 753-761. (1999: 1.090 - IF). ISSN 0009-8558.

Citácie:

1. [1.1] SWAYZE, Gregg A. - LOWERS, Heather A. - BENZEL, William M. - CLARK, Roger N. - DRISCOLL, Rhonda L. - PERLMAN, Zac S. - HOEFEN, Todd M. - DYAR, M. Darby. Characterizing the source of potentially asbestos-bearing commercial vermiculite insulation using in situ IR spectroscopy. In AMERICAN MINERALOGIST. ISSN 0003-004X, 2018, vol. 103, no. 4, pp.

517-549., Registrované v: WOS

ADCA245 MADEJOVÁ, Jana, FTIR techniques in clay mineral studies. In *Vibrational Spectroscopy*, 2003, vol. 31, no. 1, p. 1-10.

Citácie:

1. [1.1] AHMED, A. - CHAKER, Y. - BELARBI, El H. - ABBAS, O. - CHOTARD, J. N. - ABASSI, H. B. - NGUYEN VAN NHIEU, A. - EL HADRI, M. - BRESSON, S. XRD and ATR/FTIR investigations of various montmorillonite clays modified by monocationic and dicationic imidazolium ionic liquids. In *JOURNAL OF MOLECULAR STRUCTURE*. ISSN 0022-2860, 2018, vol. 1173, no., pp. 653-664., Registrované v: WOS
2. [1.1] AKYUZ, Sevim - AKYUZ, Tanil. Investigation of adsorption of 5-Chlorouracil onto montmorillonite: An IR and Raman spectroscopic study. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 164, no., pp. 54-57., Registrované v: WOS
3. [1.1] ALEXANDER, Jock Asanja - ZAINI, Muhammad Abbas Ahmad - ABDULSALAM, Surajudeen - EL-NAFATY, Usman Aliyu - AROKE, Umar Omeiza. Physicochemical characteristics of surface modified Dijah-Monkin bentonite. In *PARTICULATE SCIENCE AND TECHNOLOGY*. ISSN 0272-6351, 2018, vol. 36, no. 3, pp. 287-297., Registrované v: WOS
4. [1.1] ALSALME, Ali - ALSHARIF, Aliyah A. - AL-ENIZI, Hamda - KHAN, Mujeeb - ALSHAMMARI, Saad G. - ALOTAIBI, Mshari A. - KHAN, Rais Ahmad - SIDDIQI, Mohammed Rafiq H. Probing the Catalytic Efficiency of Supported Heteropoly Acids for Esterification: Effect of Weak Catalyst Support Interactions. In *JOURNAL OF CHEMISTRY*. ISSN 2090-9063, 2018, vol., no., pp., Registrované v: WOS
5. [1.1] ANTONIO CECILIA, Juan - PARDO, Laura - POZO, Manuel - BELLIDO, Eva - FRANCO, Francisco. Microwave-Assisted Acid Activation of Clays Composed of 2:1 Clay Minerals: A Comparative Study. In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 9, pp., Registrované v: WOS
6. [1.1] AUTIE-PEREZ, Miguel - INFANTES-MOLINA, Antonia - ANTONIO CECILIA, Juan - LABADIE-SUAREZ, Juan M. - RODRIGUEZ-CASTELLON, Enrique. Separation of Light Liquid Paraffin C-5-C-9 with Cuban Volcanic Glass Previously Used in Copper Elimination from Water Solutions. In *APPLIED SCIENCES-BASEL*. ISSN 2076-3417, 2018, vol. 8, no. 2, pp., Registrované v: WOS
7. [1.1] BASGA, Simon Djakba - TSOZUE, Desire - TEMGA, Jean Pierre - BALNA, Jules - NGUETNKAM, Jean Pierre. Land use impact on clay dispersion/flocculation in irrigated and flooded vertisols from Northern Cameroon. In *INTERNATIONAL SOIL AND WATER CONSERVATION RESEARCH*. ISSN 2095-6339, 2018, vol. 6, no. 3, pp. 237-244., Registrované v: WOS
8. [1.1] BAZILEVSKAYA, Ekaterina - ARCHIBALD, Douglas D. - MARTINEZ, Carmen Enid. Mineral colloids mediate organic carbon accumulation in a temperate forest Spodosol: depth-wise changes in pore water chemistry. In *BIOGEOCHEMISTRY*. ISSN 0168-2563, 2018, vol. 141, no. 1, pp. 75-94., Registrované v: WOS
9. [1.1] BELBEL, Abdeljabbar - KHARROUBI, Mohamed - JANOT, Jean-Marc - ABDESSAMAD, Mouffok - HAOUZI, Ahmed - LEFKAIER, Ibn Khaldoun - BALME, Sebastien. Preparation and characterization of homoionic montmorillonite modified with ionic liquid: Application in dye adsorption. In *COLLOIDS AND SURFACES A-PHYSICOCHEMICAL AND ENGINEERING ASPECTS*. ISSN 0927-7757, 2018, vol. 558, no., pp. 219-227., Registrované v: WOS
10. [1.1] BELMOKHTAR, Noureddine - EL AYADI, Houda - AMMARI, Mohammed - BEN ALLAL, Laila. Effect of structural and textural properties of a ceramic industrial sludge and kaolin on the hardened geopolymer properties. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 162, no., pp. 1-9., Registrované v: WOS
11. [1.1] BEN MOSHE, Shany - RYTWO, Giora. Thiamine-based organoclay for phenol removal from water. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 155, no., pp. 50-56., Registrované v: WOS
12. [1.1] BEN SALAH, Imed - SDIRI, Ali - JEMAI, Moufida Ben M'barek - BOUGHDIRI, Mabrouk. Potential use of the lower cretaceous clay (Kef area, Northwestern Tunisia) as raw material to supply ceramic industry. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 161, no., pp. 151-162., Registrované v: WOS
13. [1.1] BERMUDEZ, Yanisleidys Hernandez - TRUFFAULT, Laurianne - PULCINELLI, Sandra Helena - SANTILLI, Celso Valentim. Sodium montmorillonite/ureasil-poly(oxyethylene) nanocomposite as potential adsorbent of cationic dye. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 152, no., pp. 158-165., Registrované v: WOS
14. [1.1] CAROSIO, Federico - DI PIERRO, Alessandro - ALONGI, Jenny - FINA, Alberto - SARACCO, Guido. Controlling the melt dripping of polyester fabrics by tuning the ionic strength of polyhedral oligomeric silsesquioxane and sodium montmorillonite coatings assembled through Layer by Layer. In *JOURNAL OF COLLOID AND INTERFACE SCIENCE*. ISSN 0021-9797, 2018, vol. 510, no., pp. 142-151., Registrované v: WOS
15. [1.1] CASTRILLO, Natalia - MERCADO, Adela - VOLZONE, Cristina. Influence of calcium in moisture retention clay. In *MATERIA-RIO DE JANEIRO*. ISSN 1517-7076, 2018, vol. 23, no. 2, pp., Registrované v: WOS
16. [1.1] CECILIA, J. A. - GARCIA-SANCHO, C. - VILARRASA-GARCIA, E. - JIMENEZ-JIMENEZ, J. - RODRIGUEZ-CASTELLON, E. Synthesis, Characterization, Uses and Applications of Porous Clays Heterostructures: A Review. In *CHEMICAL RECORD*. ISSN 1527-8999, 2018, vol. 18, no. 7-8, pp. 1085-1104., Registrované v: WOS
17. [1.1] CECILIA, J. A. - VILARRASA-GARCIA, E. - CAVALCANTE, C. L. - AZEVEDO, D. C. S. - FRANCO, F. - RODRIGUEZ-CASTELLON, E. Evaluation of two fibrous clay minerals (sepiolite and palygorskite) for CO₂ Capture. In *JOURNAL OF ENVIRONMENTAL CHEMICAL ENGINEERING*. ISSN 2213-2929, 2018, vol. 6, no. 4, pp. 4573-4587., Registrované v: WOS
18. [1.1] CELEDON, Salvador - DE CAMARGO, Andrea S. S. - FUENTEALBA, Mauricio - ARTIGAS, Vania - BENAVENTE, Eglantina - GONZALEZ, Guillermo. Highly emissive host-guest based on nanoclay intercalated with an Eu³⁺ complex bearing a new Ru²⁺ organometallic ligand. In *NEW JOURNAL OF CHEMISTRY*. ISSN 1144-0546, 2018, vol. 42, no. 18, pp. 15284-15294., Registrované v: WOS
19. [1.1] CHARGUI, H. - HAJJAJI, W. - WOUTERS, J. - YANS, J. - JAMOSSI, F. Direct Orange 34 dye fixation by modified kaolin. In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 2, pp. 271-287., Registrované v: WOS
20. [1.1] CHAUHAN, Rohini - KUMAR, Raj - SHARMA, Vishal. Soil forensics: A spectroscopic examination of trace evidence. In *MICROCHEMICAL JOURNAL*. ISSN 0026-265X, 2018, vol. 139, no., pp. 74-84., Registrované v: WOS
21. [1.1] CHEN, Dong - WANG, Linlin - CHEN, Xiaopeng - WEI, Xiaojie - LIANG, Jiezhen - JIANG, Jiao - LIANG, Baofang. A Ni-based catalyst with polyvinyl pyrrolidone as a dispersant supported in a pretreated fluid catalytic cracking catalyst residue for C₉ petroleum resin (C₉ PR) hydrogenation. In *ROYAL SOCIETY OPEN SCIENCE*. ISSN 2054-5703, 2018, vol. 5, no. 5, pp., Registrované v: WOS

22. [1.1] CHEN, Na - SHANG, Huan - TAO, Shuangyi - WANG, Xiaobing - ZHAN, Guangming - LI, Hao - AN, Zhihui - YANG, Jiakuan - ZHANG, Lizhi. Visible Light Driven Organic Pollutants Degradation with Hydrothermally Carbonized Sewage Sludge and Oxalate Via Molecular Oxygen Activation. In ENVIRONMENTAL SCIENCE & TECHNOLOGY. ISSN 0013-936X, 2018, vol. 52, no. 21, pp. 12656-12666., Registrované v: WOS
23. [1.1] CHEN, Shuling - HONG, Hanlie - HUANG, Xianyu - FANG, Qian - YIN, Ke - WANG, Chaowen - ZHANG, Yiming - CHENG, Liuling - ALGEO, Thomas J. The role of organo-clay associations in limiting organic matter decay: Insights from the Dajiuhu peat soil, central China. In GEODERMA. ISSN 0016-7061, 2018, vol. 320, no., pp. 149-160., Registrované v: WOS
24. [1.1] CHICINAS, R. Plesa - BEDELEAN, H. - STEFAN, R. - MAICANEANU, A. Ability of a montmorillonitic clay to interact with cationic and anionic dyes in aqueous solutions. In JOURNAL OF MOLECULAR STRUCTURE. ISSN 0022-2860, 2018, vol. 1154, no., pp. 187-195., Registrované v: WOS
25. [1.1] CONSELVAN, Giovanni Battista - FUENTES, David - MERCHANT, Andrew - PEGGION, Cristina - FRANCIOSO, Ornella - CARLETTI, Paolo. Effects of humic substances and indole-3-acetic acid on Arabidopsis sugar and amino acid metabolic profile. In PLANT AND SOIL. ISSN 0032-079X, 2018, vol. 426, no. 1-2, pp. 17-32., Registrované v: WOS
26. [1.1] D'ELIA, A. - PINTO, D. - ERAMO, G. - GIANNOSSA, L. C. - VENTRUTI, G. - LAVIANO, R. Effects of processing on the mineralogy and solubility of carbonate-rich clays for alkaline activation purpose: mechanical, thermal activation in red/ox atmosphere and their combination. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 152, no., pp. 9-21., Registrované v: WOS
27. [1.1] DANNER, Tobias - NORDEN, Geir - JUSTNES, Harald. Characterisation of calcined raw clays suitable as supplementary cementitious materials. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 162, no., pp. 391-402., Registrované v: WOS
28. [1.1] EL-HABAAK, Galal - ASKALANY, Mohamed - ABDEL-HAKEEM, Mahmoud. The effect of mineralogy of calcined shales on the alkali activation and geopolymerization reactions: A case study from Abu-Tartur plateau, Western Desert, Egypt. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 162, no., pp. 90-100., Registrované v: WOS
29. [1.1] FERNANDEZ, A. M. - KAUFHOLD, S. - SANCHEZ-LEDESMA, D. M. - REY, J. J. - MELON, A. - ROBREDO, L. M. - FERNANDEZ, S. - LABAJO, M. A. - CLAVERO, M. A. Evolution of the THC conditions in the FEBEX in situ test after 18 years of experiment: Smectite crystallochemical modifications after interactions of the bentonite with a C-steel heater at 100 degrees C. In APPLIED GEOCHEMISTRY. ISSN 0883-2927, 2018, vol. 98, no., pp. 152-171., Registrované v: WOS
30. [1.1] FORTE, Vanessa - CESARO, Stella Nunziante - MEDEGHINI, Laura. Cooking traces on Copper Age pottery from central Italy: An integrated approach comprising use wear analysis, spectroscopic analysis and experimental archaeology. In JOURNAL OF ARCHAEOLOGICAL SCIENCE-REPORTS. ISSN 2352-409X, 2018, vol. 18, no., pp. 121-138., Registrované v: WOS
31. [1.1] FREITAS, Renato P. - COELHO, Filipe A. - FELIX, Valter S. - PEREIRA, Marcelo O. - TORRES DE SOUZA, Marcos Andre - ANJOS, Marcelino J. Analysis of 19th century ceramic fragments excavated from Pirenopolis (Goiás, Brazil) using FT-IR, Raman, XRF and SEM. In SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY. ISSN 1386-1425, 2018, vol. 193, no., pp. 432-439., Registrované v: WOS
32. [1.1] GAL, Agnes - IONESCU, Corina - BAJUSZ, Matyas - CODREA, Vlad A. - HOECK, Volker - BARBUTUDORAN, Lucian - SIMON, Viorica - MURESAN-POP, Marieta - CSOK, Zsolt. Composition, technology and provenance of Roman pottery from Napoca (Cluj-Napoca, Romania). In CLAY MINERALS. ISSN 0009-8558, 2018, vol. 53, no. 4, pp. 621-641., Registrované v: WOS
33. [1.1] GANGULY, Sayan - MONDAL, Subhadip - DAS, Poushali - BHAWAL, Poushali - MAITY, Priti Prasanna - GHOSH, Sabyasachi - DHARA, Santanu - DAS, Narayan Ch. Design of psyllium-g-poly(acrylic acid-co-sodium acrylate)/cloisite 10A semi-IPN nanocomposite hydrogel and its mechanical, rheological and controlled drug release behaviour. In INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES. ISSN 0141-8130, 2018, vol. 111, no., pp. 983-998., Registrované v: WOS
34. [1.1] GHOFUR, Abdul - SOEMARNO - HADI, Abdul - PUTRA, Meilana Dharma. Potential fly ash waste as catalytic converter for reduction of HC and CO emissions. In SUSTAINABLE ENVIRONMENT RESEARCH. ISSN 2468-2039, 2018, vol. 28, no. 6, pp. 357-362., Registrované v: WOS
35. [1.1] GONZALEZ-RAYMAT, Hansell - ANAGNOSTOPOULOS, Vasileios - DENHAM, Miles - CAI, Yong - KATSENOVICH, Yelena P. Unrefined humic substances as a potential low-cost amendment for the management of acidic groundwater contamination. In JOURNAL OF ENVIRONMENTAL MANAGEMENT. ISSN 0301-4797, 2018, vol. 212, no., pp. 210-218., Registrované v: WOS
36. [1.1] GYOLLAI, Ildiko - POLGARI, Marta - BIRO, Lorant - VIGH, Tamas - KOVACS, Tibor - PAL-MOLNAR, Elemer. FOSSILIZED BIOMATS AS THE POSSIBLE SOURCE OF HIGH NATURAL RADIONUCLIDE CONTENT AT THE JURASSIC URKUT MANGANESE ORE DEPOSIT, HUNGARY. In CARPATHIAN JOURNAL OF EARTH AND ENVIRONMENTAL SCIENCES. ISSN 1842-4090, 2018, vol. 13, no. 2, pp. 477-487., Registrované v: WOS
37. [1.1] HAHN, Annette - VOGEL, Hendrik - ANDO, Sergio - GARZANTI, Eduardo - KUHN, Gerhard - LANTZSCH, Hendrik - SCHUEUERMAN, Jan - VOGT, Christoph - ZABEL, Matthias. Using Fourier transform infrared spectroscopy to determine mineral phases in sediments. In SEDIMENTARY GEOLOGY. ISSN 0037-0738, 2018, vol. 375, no., pp. 27-35., Registrované v: WOS
38. [1.1] HONG, Lei - ROMANOV, Vyacheslav. Experimental Studies: Molecular Interactions at Clay Interfaces. In GREENHOUSE GASES AND CLAY MINERALS: ENLIGHTENING DOWN-TO-EARTH ROAD MAP TO BASIC SCIENCE OF CLAY-GREENHOUSE GAS INTERFACES. ISSN 1865-3529, 2018, vol., no., pp. 95-123., Registrované v: WOS
39. [1.1] HRADIL, David - HRADILOVA, Janka - HOLCOVA, Katarina - BEZDICKA, Petr. The use of pottery clay for canvas priming in Italian Baroque An example of technology transfer. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 165, no., pp. 135-147., Registrované v: WOS
40. [1.1] HUANG, Yang - DENG, Jie - WANG, Weiqing - FENG, Qiming - XU, Zhonghui. Preliminary Investigation of Pozzolan Properties of Calcined Waste Kaolin. In MATERIALS SCIENCE-MEDZIAGOTYRA. ISSN 1392-1320, 2018, vol. 24, no. 2, pp. 177-184., Registrované v: WOS
41. [1.1] HUO, Mingyuan - GUO, Honggang - JIANG, Yinshan - JU, Hao - XUE, Bing - LI, Fangfei. A facile method of preparing sandwich layered TiO₂ in between montmorillonite sheets and its enhanced UV-light photocatalytic activity. In JOURNAL OF

- PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY*. ISSN 1010-6030, 2018, vol. 358, no., pp. 121-129., Registrované v: WOS
42. [1.1] JIANG, Jun - CAO, Jinzhen - WANG, Wang - MEI, Changtong. Analysis on the Influence of Component Ratio on Properties of Silica/Montmorillonite Nanocomposites. In *MATERIALS*. ISSN 1996-1944, 2018, vol. 11, no. 11, pp., Registrované v: WOS
43. [1.1] JU, Hao - JIANG, Yinshan - XUE, Bing - XU, Yuanjun - GUO, Honggang - HUO, Mingyuan - LI, Fangfei. UV shielding performance of illite/TiO₂ nanocomposites. In *NEW JOURNAL OF CHEMISTRY*. ISSN 1144-0546, 2018, vol. 42, no. 11, pp. 9260-9268., Registrované v: WOS
44. [1.1] KAYNAR, Umit H. - HICSONMEZ, Umran - KAYNAR, Sermin Cam - KOCAK, Suleyman. Sorption of uranium(VI) from aqueous solutions by DEEA organo-volcanic: isotherms, kinetic and thermodynamic studies. In *NUCLEAR SCIENCE AND TECHNIQUES*. ISSN 1001-8042, 2018, vol. 29, no. 2, pp., Registrované v: WOS
45. [1.1] KERESZTURI, Akos - FINTOR, Krisztian - GYOLLAI, Ildiko - KERESZTY, Zsolt - SZABO, Mate - SZALAI, Zoltan - WALTER, Ena. Shock heterogeneity and shock history of the recently found ordinary Csatalja chondrite in Hungary. In *GEOLOGICAL QUARTERLY*. ISSN 1641-7291, 2018, vol. 62, no. 2, pp. 433-446., Registrované v: WOS
46. [1.1] KHABBOUCHI, M. - HOSNI, K. - SRASRA, E. Physico-Chemical Characterization of Modified Tunisian Kaolin by Phosphoric Acid. In *SURFACE ENGINEERING AND APPLIED ELECTROCHEMISTRY*. ISSN 1068-3755, 2018, vol. 54, no. 2, pp. 219-226., Registrované v: WOS
47. [1.1] KHABBOUCHI, Mohamed - HOSNI, Khaled - MEZNI, Mohamed - SRASRA, Ezzeddine. Simplified synthesis of silicophosphate materials using an activated metakaolin as a natural source of active silica. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 158, no., pp. 169-176., Registrované v: WOS
48. [1.1] KHABBOUCHI, Mohamed - HOSNI, Khaled - SRASRA, Ezzeddine. Structural, Textural and Mechanical Properties of Products Obtained by Interaction of Metakaolin-phosphoric Acid at High Temperature. In *RUSSIAN JOURNAL OF APPLIED CHEMISTRY*. ISSN 1070-4272, 2017, vol. 90, no. 12, pp. 2046-2054., Registrované v: WOS
49. [1.1] KIM, Aran - RYU, Seung-Jin - LEE, Jihye - JUNG, Hyun. Development of Latent Fingermarks on Nonporous and Semiporous Substrates Using Photoluminescent Eu(Phen)(2) Complex Intercalated Clay Hybrids with Enhanced Adhesion. In *JOURNAL OF FORENSIC SCIENCES*. ISSN 0022-1198, 2018, vol. 63, no. 6, pp. 1718-1726., Registrované v: WOS
50. [1.1] LANDRE, A. - SABY, N. P. A. - BARTHE, B. G. - RATIE, C. - GUERIN, A. - ETAYO, A. - MINASNY, B. - BARDY, M. - MEUNIER, J.D. - CORNU, S. Prediction of total silicon concentrations in French soils using pedotransfer functions from mid-infrared spectrum and pedological attributes. In *GEODERMA*. ISSN 0016-7061, 2018, vol. 331, no., pp. 70-80., Registrované v: WOS
51. [1.1] LI, Wenyun - BAI, Yunshan - MA, Qingliang - CHEN, Wenjuan - WU, Min - MA, Hongzhu. Polyacrylic acid/CTAB-bentonite coated filter paper: Efficient and rapid removal of anionic and cationic dyes. In *APPLIED SURFACE SCIENCE*. ISSN 0169-4332, 2018, vol. 458, no., pp. 903-909., Registrované v: WOS
52. [1.1] LI, Wenyun - MA, Qingliang - BAI, Yunshan - XU, Dandan - WU, Min - MA, Hongzhu. Facile fabrication of gelatin/bentonite composite beads for tunable removal of anionic and cationic dyes. In *CHEMICAL ENGINEERING RESEARCH & DESIGN*. ISSN 0263-8762, 2018, vol. 134, no., pp. 336-346., Registrované v: WOS
53. [1.1] LIN, Jing - LUO, Yuanfang - ZHONG, Bangchao - HU, Dechao - JIA, Zhixin - JIA, Demin. Enhanced interfacial interaction and antioxidative behavior of novel halloysite nanotubes/silica hybrid supported antioxidant in styrene-butadiene rubber. In *APPLIED SURFACE SCIENCE*. ISSN 0169-4332, 2018, vol. 441, no., pp. 798-806., Registrované v: WOS
54. [1.1] LIU, Jie - WANG, Xue-Qian - YANG, Bei-Bei - LIU, Chun-Ling - XU, Chun-Li - DONG, Wen-Sheng. Highly efficient conversion of glucose into methyl levulinate catalyzed by tin-exchanged montmorillonite. In *RENEWABLE ENERGY*. ISSN 0960-1481, 2018, vol. 120, no., pp. 231-240., Registrované v: WOS
55. [1.1] LIU, Wei - ZHAO, Chenchen - WANG, Shutao - NIU, Lin - WANG, Yunli - LIANG, Shuxuan - CUI, Zhe. Adsorption of cadmium ions from aqueous solutions using nano-montmorillonite: kinetics, isotherm and mechanism evaluations. In *RESEARCH ON CHEMICAL INTERMEDIATES*. ISSN 0922-6168, 2018, vol. 44, no. 3, pp. 1441-1458., Registrované v: WOS
56. [1.1] LIU, Xueping - WU, Xuantao - WANG, Jie. Substantial upgrading of a high-ash lignite by hydrothermal treatment followed by Ca(OH)₂ digestion/acid leaching. In *FUEL*. ISSN 0016-2361, 2018, vol. 222, no., pp. 269-277., Registrované v: WOS
57. [1.1] LONG, Zheru - WU, Yan-Ping - GAO, Hua-Ying - ZHANG, Jun - OU, Xianfeng - HE, Rong-Rong - LIU, Mingxian. In vitro and in vivo toxicity evaluation of halloysite nanotubes. In *JOURNAL OF MATERIALS CHEMISTRY B*. ISSN 2050-750X, 2018, vol. 6, no. 44, pp. 7204-7216., Registrované v: WOS
58. [1.1] LORENTZ, Brandon - SHANAHAN, Natallia - STETSKO, Yuri P. - ZAYED, A. Characterization of Florida kaolin clays using multiple-technique approach. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 161, no., pp. 326-333., Registrované v: WOS
59. [1.1] MAHMOODI, Syed Muhammad Ibad - PADMANABHAN, Eswaran. Hydrocarbon Bond Variation in Some Shales from Batu Gajah, Malaysia. In *ICIPEG 2016: PROCEEDINGS OF THE INTERNATIONAL CONFERENCE ON INTEGRATED PETROLEUM ENGINEERING AND GEOSCIENCES*, 2017, vol., no., pp. 363-371., Registrované v: WOS
60. [1.1] MALAKOOTIAN, Mohammad - HOSSAINI, Hiwa - ASADIPOUR, Ali - DANESHKHAH, Mozghan. Preparation and characterization of modified sepiolite for the removal of Acid green 20 from aqueous solutions: isotherm, kinetic and process optimization. In *APPLIED WATER SCIENCE*. ISSN 2190-5487, 2018, vol. 8, no. 6, pp., Registrované v: WOS
61. [1.1] MENG, Jie - LIU, Xiaoyang - LI, Benxian - ZHANG, Juncheng - HU, Daqian - CHEN, Jiuhua - SHI, Weiguang. Conversion reactions from dioctahedral smectite to trioctahedral chlorite and their structural simulations. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 158, no., pp. 252-263., Registrované v: WOS
62. [1.1] MIDDEA, Antonietta - SPINELLI, Luciana - DE SOUZA JUNIOR, Fernando Gomes - NEUMANN, Reiner - FERNANDES, Thais - LEITE FAULSTICH, Fabiano Richard - GOMES, Otavio. Magnetic polystyrene-palygorskite nanocomposite obtained by heterogeneous phase polymerization to apply in the treatment of oily waters. In *JOURNAL OF APPLIED POLYMER SCIENCE*. ISSN 0021-8995, 2018, vol. 135, no. 15, pp., Registrované v: WOS
63. [1.1] MORADI, Neshat - SALEM, Shiva - SALEM, Amin. Optimizing adsorption of blue pigment from wastewater by nano-

- porous modified Na-bentonite using spectrophotometry based on response surface method. In *SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY*. ISSN 1386-1425, 2018, vol. 193, no., pp. 54-62., Registrované v: WOS
64. [1.1] NADJI, L. - MASSO, A. - DELGADO, D. - ISSAADI, R. - RODRIGUEZ-AGUADO, E. - RODRIGUEZ-CASTELLON, E. - LOPEZ NIETO, J. M. Gas phase dehydration of glycerol to acrolein over WO₃-based catalysts prepared by non-hydrolytic sol-gel synthesis. In *RSC ADVANCES*. ISSN 2046-2069, 2018, vol. 8, no. 24, pp. 13344-13352., Registrované v: WOS
65. [1.1] NATSIR, Taufik Abdillah - HARA, Takayoshi - ICHIKUNI, Nobuyuki - SHIMAZU, Shogo. Kaolinite Catalyst for the Production of a Biodiesel-Based Compound from Biomass-Derived Furfuryl Alcohol. In *ACS APPLIED ENERGY MATERIALS*. ISSN 2574-0962, 2018, vol. 1, no. 6, pp. 2460-2463., Registrované v: WOS
66. [1.1] NDZANA, Georges Martial - HUANG, Li - WANG, Jin Bo - ZHANG, Zhi Yi. Characteristics of clay minerals in soil particles from an argillic horizon of Alfisol in central China. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 151, no., pp. 148-156., Registrované v: WOS
67. [1.1] NOOR, Norhayati Mohd - SOI, Hoong Seng - ISMAIL, Tuan Noor Maznee Tuan - HANZAH, Nurul Ain - KIAN, Yeong Shoot - IDRIS, Zainab. PERFORMANCE OF RECYCLED K10 MONTMORILLONITE CATALYST IN THE ALCOHOLYSIS OF EPOXIDISED PALM OLEIN. In *JOURNAL OF OIL PALM RESEARCH*. ISSN 1511-2780, 2018, vol. 30, no. 2, pp. 326-337., Registrované v: WOS
68. [1.1] PARDO, Laura - ANTONIO CECILIA, Juan - LOPEZ-MORENO, Cristina - HERNANDEZ, Victor - POZO, Manuel - JOSE BENTABOL, Maria - FRANCO, Francisco. Influence of the Structure and Experimental Surfaces Modifications of 2:1 Clay Minerals on the Adsorption Properties of Methylene Blue. In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 8, pp., Registrované v: WOS
69. [1.1] PELAYO, M. - MARCO, J. F. - FERNANDEZ, A. M. - VERGARA, L. - MELON, A. M. - PEREZ DEL VILLAR, L. Infrared and Mossbauer spectroscopy of Fe-rich smectites from Morron de Mateo bentonite deposit (Spain). In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 1, pp. 17-28., Registrované v: WOS
70. [1.1] PEYNE, Julie - GHARZOUNI, Ameni - SOBRADOS, Isabel - ROSSIGNOL, Sylvie. Identifying the differences between clays used in the brick industry by various methods: Iron extraction and NMR spectroscopy. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 160, no., pp. 290-298., Registrované v: WOS
71. [1.1] PURI, Chandni - SUMANA, Gajjala. Highly effective adsorption of crystal violet dye from contaminated water using graphene oxide intercalated montmorillonite nanocomposite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 166, no., pp. 102-112., Registrované v: WOS
72. [1.1] RAHMAN, M. R. - HAMDAN, S. - LAI, J. C. H. Preparation and Characterizations of Clay-Dispersed Styrene-co-Ethylene Glycol Dimethacrylate-Impregnated Wood Polymer Nanocomposites. In *WOOD POLYMER NANOCOMPOSITES: CHEMICAL MODIFICATIONS, PROPERTIES AND SUSTAINABLE APPLICATIONS*. ISSN 1612-1317, 2018, vol., no., pp. 199-217., Registrované v: WOS
73. [1.1] RAMASAMY, V. - ANAND, P. - SURESH, G. Synthesis and characterization of polymer-mediated CaCO₃ nanoparticles using limestone: A novel approach. In *ADVANCED POWDER TECHNOLOGY*. ISSN 0921-8831, 2018, vol. 29, no. 3, pp. 818-834., Registrované v: WOS
74. [1.1] RANGEL-PORRAS, Gustavo - MONCADA-SANCHEZ, Cristina - ZARRAGA-NUNEZ, Ramon - ROMERO-TOLEDO, Rafael - MIRANDA-AVILES, Raul. Thermogravimetric characterization of tyrosine and catechol adsorbed on montmorillonite. In *INSTRUMENTATION SCIENCE & TECHNOLOGY*. ISSN 1073-9149, 2018, vol. 46, no. 6, pp. 676-692., Registrované v: WOS
75. [1.1] RANGEL-RIVERA, Pedro - BELEN BACHILLER-BAEZA, Maria - GALINDO-ESQUIVEL, Ignacio - RANGEL-PORRAS, Gustavo. Inclusion of Ti and Zr species on clay surfaces and their effect on the interaction with organic molecules. In *APPLIED SURFACE SCIENCE*. ISSN 0169-4332, 2018, vol. 445, no., pp. 229-241., Registrované v: WOS
76. [1.1] RAUSCHER, Markus S. - SCHARDT, Michael - KOEHLER, Michael H. - KOCH, Alexander W. Dual-channel mid-infrared sensor based on tunable Fabry-Perot filters for fluid monitoring applications. In *SENSORS AND ACTUATORS B-CHEMICAL*. ISSN 0925-4005, 2018, vol. 259, no., pp. 420-427., Registrované v: WOS
77. [1.1] RENNERT, Thilo - GEORGIADIS, Anna - GHONG, Nchia Peter - RINKLEBE, Joerg. Compositional variety of soil organic matter in mollic floodplain-soil profiles Also an indicator of pedogenesis. In *GEODERMA*. ISSN 0016-7061, 2018, vol. 311, no., pp. 15-24., Registrované v: WOS
78. [1.1] RIBEIRO, Halisson L. - BRITO, Edy S. - SOUZA FILHO, Men de sa M. - AZEREDO, Henriette M. C. Montmorillonite as a reinforcement and color stabilizer of gelatin films containing acerola juice. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 165, no., pp. 1-7., Registrované v: WOS
79. [1.1] RIBEIRO, Halisson L. - DE OLIVEIRA, Ana Vitoria - DE BRITO, Edy S. - RIBEIRO, Paulo R. V. - SOUZA FILHO, Men de Sa M. - AZEREDO, Henriette M. C. Stabilizing effect of montmorillonite on acerola juice anthocyanins. In *FOOD CHEMISTRY*. ISSN 0308-8146, 2018, vol. 245, no., pp. 966-973., Registrované v: WOS
80. [1.1] RITZ, Michal - VALASKOVA, Marta. Infrared and Raman spectroscopy of three commercial vermiculites doped with cerium dioxide nanoparticles. In *SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY*. ISSN 1386-1425, 2018, vol. 201, no., pp. 39-45., Registrované v: WOS
81. [1.1] ROCA JALIL, Maria Eugenia - TOSCHI, Florencia - BASCHINI, Miria - SAPAG, Karim. Silica Pillared Montmorillonites as Possible Adsorbents of Antibiotics from Water Media. In *APPLIED SCIENCES-BASEL*. ISSN 2076-3417, 2018, vol. 8, no. 8, pp., Registrované v: WOS
82. [1.1] ROCHA, Mariana - COSTA, Paula - SOUSA, Carlos A. D. - PEREIRA, Clara - RODRIGUEZ-BORGES, Jose E. - FREIRE, Cristina. L-serine-functionalized montmorillonite decorated with Au nanoparticles: A new highly efficient catalyst for the reduction of 4-nitrophenol. In *JOURNAL OF CATALYSIS*. ISSN 0021-9517, 2018, vol. 361, no., pp. 143-155., Registrované v: WOS
83. [1.1] ROMANOV, Vyacheslav. Advanced Experimental Techniques in Geochemistry. In *GREENHOUSE GASES AND CLAY MINERALS: ENLIGHTENING DOWN-TO-EARTH ROAD MAP TO BASIC SCIENCE OF CLAY-GREENHOUSE GAS INTERFACES*. ISSN 1865-3529, 2018, vol., no., pp. 77-94., Registrované v: WOS
84. [1.1] RUAN, Bo - WU, Pingxiao - LAI, Xiaolin - WANG, Huimin - LI, Liping - CHEN, Liya - KANG, Chunxi - ZHU, Nengwu - DANG, Zhi - LU, Guining. Effects of *Sphingomonas* sp GY2B on the structure and physicochemical properties of stearic acid-

- modified montmorillonite in the biodegradation of phenanthrene. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 156, no., pp. 36-44., Registrované v: WOS
85. [1.1] RUAN, Bo - WU, Pingxiao - WANG, Huimin - LI, Liping - YU, Langfeng - CHEN, Liya - LAI, Xiaolin - ZHU, Nengwu - DANG, Zhi - LU, Guining. Effects of interaction between montmorillonite and *Sphingomonas* sp GY2B on the physical and chemical properties of montmorillonite in the clay-modulated biodegradation of phenanthrene. In *ENVIRONMENTAL CHEMISTRY*. ISSN 1448-2517, 2018, vol. 15, no. 5, pp. 296-305., Registrované v: WOS
86. [1.1] SAID, Muhammad - UTAMI, Hasja Paluta - HAYATI, Ferlina. Insertion of bentonite with Organometallic [Fe3O(OOC6H5)(6)(H2O)(3)(NO3)center dot nH(2)O] as Adsorbent of Congo Red. In *INTERNATIONAL CONFERENCE ON CHEMISTRY AND MATERIAL SCIENCE (IC2MS) 2017*. ISSN 1757-8981, 2018, vol. 299, no., pp., Registrované v: WOS
87. [1.1] SALEHI, Tahereh Mombeini - PEYRAVI, Majid - JAHANSHAH, Mohsen - LAU, Woei-Jye - RAD, Ali Shokuhi. Impacts of zeolite nanoparticles on substrate properties of thin film nanocomposite membranes for engineered osmosis. In *JOURNAL OF NANOPARTICLE RESEARCH*. ISSN 1388-0764, 2018, vol. 20, no. 4, pp., Registrované v: WOS
88. [1.1] SAMANI, Faranak - BAHRAMIAN, Ahmad Reza - SHARIF, Alireza. Shape-stable phenolic/polyethylene glycol phase change material: kinetics study and improvements in thermal properties of nanocomposites. In *IRANIAN POLYMER JOURNAL*. ISSN 1026-1265, 2018, vol. 27, no. 7, pp. 495-505., Registrované v: WOS
89. [1.1] SARMA, Gautam Kumar - SENGUPTA, Susmita - BHATTACHARYA, Krishna G. Adsorption of Monoazo Dyes (Crocein Orange G and Procion Red MX5B) from Water Using Raw and Acid-Treated Montmorillonite K10: Insight into Kinetics, Isotherm, and Thermodynamic Parameters. In *WATER AIR AND SOIL POLLUTION*. ISSN 0049-6979, 2018, vol. 229, no. 10, pp., Registrované v: WOS
90. [1.1] SHATTAR, S. F. A. - ZAKARIA, N. A. - FOO, K. Y. Acid modified natural clay as a judicious solution for the successive treatment of ametryn. In *DESALINATION AND WATER TREATMENT*. ISSN 1944-3994, 2018, vol. 103, no., pp. 270-279., Registrované v: WOS
91. [1.1] SILVA, Dafenes B. R. dos S. - JUNIOR, Lindemberg P. C. - DE AGUIAR, Mauricio F. - DE MELO, Celso P. - ALVES, Kleber G. B. Preparation and characterization of nanofibers of polyvinyl alcohol/polyaniline-montmorillonite clay. In *JOURNAL OF MOLECULAR LIQUIDS*. ISSN 0167-7322, 2018, vol. 272, no., pp. 1070-1076., Registrované v: WOS
92. [1.1] SONG, Chao - ZHOU, Yuan-yuan - LIU, Quan-jun - DENG, Jian-ying - LI, Shi-mei - GAO, Li-kun - YU, Li. Effects of BaCl2 on K-feldspar flotation using dodecyl amine chloride under natural pH. In *TRANSACTIONS OF NONFERROUS METALS SOCIETY OF CHINA*. ISSN 1003-6326, 2018, vol. 28, no. 11, pp. 2335-2341., Registrované v: WOS
93. [1.1] SRIVASTAVA, Priyeshu - SIDDIAH, N. Siva - SANGODE, S. J. - MESHRAM, D. C. Mineralogy and geochemistry of various colored boles from the Deccan volcanic province: Implications for paleoweathering and paleoenvironmental conditions. In *CATENA*. ISSN 0341-8162, 2018, vol. 167, no., pp. 44-59., Registrované v: WOS
94. [1.1] STAWINSKI, Wojciech - WEGRZYŃ, Agnieszka - MORDARSKI, Grzegorz - SKIBA, Michał - FREITAS, Olga - FIGUEIREDO, Sonia. Sustainable adsorbents formed from by-product of acid activation of vermiculite and leached-vermiculite-LDH hybrids for removal of industrial dyes and metal cations. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 161, no., pp. 6-14., Registrované v: WOS
95. [1.1] STEMPFLE, Sabrina - LINSTAEDTER, Joerg - NICKEL, Klaus G. - MIKDDAD, Abdeslam - SCHMIDT, Patrick. Early Neolithic pottery of Ifri n'etsedda, NE-Morocco Raw materials and fabrication techniques. In *JOURNAL OF ARCHAEOLOGICAL SCIENCE-REPORTS*. ISSN 2352-409X, 2018, vol. 19, no., pp. 200-212., Registrované v: WOS
96. [1.1] SULTAN, Md. Tipu - RAHMAN, Md. Rezaur - HAMDAN, Sinin - HOSSEN, Md. Faruk - MAZLAN, Amaliah Binti. Improved Interfacial Interaction between Wood and Styrene with the Help of Organically Modified Nanoclay. In *BIORESOURCES*. ISSN 1930-2126, 2018, vol. 13, no. 4, pp. 8100-8112., Registrované v: WOS
97. [1.1] SWAYZE, Gregg A. - LOWERS, Heather A. - BENZEL, William M. - CLARK, Roger N. - DRISCOLL, Rhonda L. - PERLMAN, Zac S. - HOEFEN, Todd M. - DYAR, M. Darby. Characterizing the source of potentially asbestos-bearing commercial vermiculite insulation using in situ IR spectroscopy. In *AMERICAN MINERALOGIST*. ISSN 0003-004X, 2018, vol. 103, no. 4, pp. 517-549., Registrované v: WOS
98. [1.1] TAVARES LUNA, Francisco Murilo - ANTONIO CECILIA, Juan - ALVES SABOYA, Rosana Maria - BARRERA, Deicy - SAPAG, Karim - RODRIGUEZ-CASTELLON, Enrique - CAVALCANTE, Celio Loureiro. Natural and Modified Montmorillonite Clays as Catalysts for Synthesis of Biolubricants. In *MATERIALS*. ISSN 1996-1944, 2018, vol. 11, no. 9, pp., Registrované v: WOS
99. [1.1] TCHOUMENE, Rolland - DEDZO, Gustave Kenne - NGAMENI, Emmanuel. Preparation of Methyl Viologen-Kaolinite Intercalation Compound: Controlled Release and Electrochemical Applications. In *ACS APPLIED MATERIALS & INTERFACES*. ISSN 1944-8244, 2018, vol. 10, no. 40, pp. 34534-34542., Registrované v: WOS
100. [1.1] TINTNER, J. - SMIDT, E. - AUMUELLER, C. - MARTIN, P. - OTTNER, F. - WRIESSNIG, K. - RESCHREITER, H. Taphonomy of prehistoric bark in a salt environment at the archaeological site in Hallstatt, Upper Austria An analytical approach based on FTIR spectroscopy. In *VIBRATIONAL SPECTROSCOPY*. ISSN 0924-2031, 2018, vol. 97, no., pp. 39-43., Registrované v: WOS
101. [1.1] TRIGUEIRO, Pollyana - PEDETTI, Silvia - RIGAUD, Baptiste - BALME, Sebastien - JANOT, Jean-Marc - DOS SANTOS, Leda M. G. - GOUGEON, Regis - FONSECA, Maria G. - GEORGELIN, Thomas - JABER, Maguy. Going through the wine fining: Intimate dialogue between organics and clays. In *COLLOIDS AND SURFACES B-BIOINTERFACES*. ISSN 0927-7765, 2018, vol. 166, no., pp. 79-88., Registrované v: WOS
102. [1.1] TSANTOS, C. - GIONIS, V. - CHRYSOSIKOS, G. D. Smectite in bentonite: Near infrared systematics and estimation of layer charge. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 160, no., pp. 81-87., Registrované v: WOS
103. [1.1] UZAROWICZ, Lukasz - SKIBA, Michał - LEUE, Martin - ZAGORSKI, Zbigniew - GASINSKI, Arkadiusz - TRZCINSKI, Jerzy. Technogenic soils (Technosols) developed from fly ash and bottom ash from thermal power stations combusting bituminous coal and lignite. Part II. Mineral transformations and soil evolution. In *CATENA*. ISSN 0341-8162, 2018, vol. 162, no., pp. 255-269., Registrované v: WOS
104. [1.1] VLASOVA, Marina - PARRA PARRA, Abigail - MARQUEZ AGUILAR, Pedro Antonio - TRUJILLO ESTRADA, Ariadna - GONZALEZ MOLINA, Veronica - KAKAZEY, Mykola - TOMILA, Tamara - GOMEZ-VIDALES, Virginia. Closed cycle of recycling of waste activated sludge. In *WASTE MANAGEMENT*. ISSN 0956-053X, 2018, vol. 71, no., pp. 320-333., Registrované v: WOS
105. [1.1] WANG, Jie - GAO, Manglai - DING, Fan - SHEN, Tao. Organo-vermiculites modified by heating and gemini pyridinium

- surfactants: Preparation, characterization and sulfamethoxazole adsorption. In *COLLOIDS AND SURFACES A-PHYSICOCHEMICAL AND ENGINEERING ASPECTS*. ISSN 0927-7757, 2018, vol. 546, no., pp. 143-152., Registrované v: WOS
106. [1.1] WANG, Ying - CHENG, Pengfei - LI, Fangbai - LIU, Tongxu - CHENG, Kuan - YANG, Jinling - LU, Ying. Variable charges of a red soil from different depths: Acid-base buffer capacity and surface complexation model. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 159, no., pp. 107-115., Registrované v: WOS
107. [1.1] WANG, Ying - HE, Hui - ZHANG, Nan - SHIMIZU, Kazuya - LEI, Zhongfang - ZHANG, Zhenya. Efficient capture of phosphate from aqueous solution using acid activated akadama clay and mechanisms analysis. In *WATER SCIENCE AND TECHNOLOGY*. ISSN 0273-1223, 2018, vol. 78, no. 7, pp. 1603-1614., Registrované v: WOS
108. [1.1] WĘGRZYN, Agnieszka - STAWINSKI, Wojciech - FREITAS, Olga - KOMEDERA, Kamila - BLACHOWSKI, Artur - JECZMIONEK, Lukasz - DANKO, Tomasz - MORDARSKI, Grzegorz - FIGUEIREDO, Sonia. Study of adsorptive materials obtained by wet fine milling and acid activation of vermiculite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 155, no., pp. 37-49., Registrované v: WOS
109. [1.1] WU, Yan-Ping - YANG, Jing - GAO, Hua-Ying - SHEN, Yan - JIANG, Lingxiang - ZHOU, Changren - LI, Yi-Fang - HE, Rong-Rong - LIU, Mingxian. Folate-Conjugated Halloysite Nanotubes, an Efficient Drug Carrier, Deliver Doxorubicin for Targeted Therapy of Breast Cancer. In *ACS APPLIED NANO MATERIALS*. ISSN 2574-0970, 2018, vol. 1, no. 2, pp. 595-608., Registrované v: WOS
110. [1.1] XIA, Meng - ZHENG, Xianming - DU, Mingyang - WANG, Yingying - DING, Aizhong - DOU, Junfeng. The adsorption of Cs⁺ from wastewater using lithium-modified montmorillonite caged in calcium alginate beads. In *CHEMOSPHERE*. ISSN 0045-6535, 2018, vol. 203, no., pp. 271-280., Registrované v: WOS
111. [1.1] XIE, Yanluo - XIAO, Kemeng - SUN, Yang - GAO, Yufeng - YANG, Han - XU, Heng. Effects of amendments on heavy metal immobilization and uptake by *Rhizoma chuanxiong* on copper and cadmium contaminated soil. In *ROYAL SOCIETY OPEN SCIENCE*. ISSN 2054-5703, 2018, vol. 5, no. 8, pp., Registrované v: WOS
112. [1.1] XU, Xiubin - LU, Shaoyu - WU, Can - WANG, Zhiyong - FENG, Chen - WEN, Na - LIU, Mingzhu - ZHANG, Xinyu - LIU, Zhen - LIU, Yongqi - REN, Chunzhen. Curcumin polymer coated, self-fluorescent and stimuli-responsive multifunctional mesoporous silica nanoparticles for drug delivery. In *MICROPOROUS AND MESOPOROUS MATERIALS*. ISSN 1387-1811, 2018, vol. 271, no., pp. 234-242., Registrované v: WOS
113. [1.1] YAN, Xiaodan - SHI, Lin - CAI, Rumeng. Improvement of nitrogen utilization and soil properties by addition of a mineral soil conditioner: mechanism and performance. In *ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH*. ISSN 0944-1344, 2018, vol. 25, no. 3, pp. 2805-2813., Registrované v: WOS
114. [1.1] YAN, Xiaodan - SHI, Lin - GONG, Lingting. Mechanism analysis of soil amelioration and phosphorus recovery by using a mineral soil conditioner in southern China. In *JOURNAL OF SOILS AND SEDIMENTS*. ISSN 1439-0108, 2018, vol. 18, no. 5, pp. 1884-1895., Registrované v: WOS
115. [1.1] YANG, Yu-Ling - REDDY, Krishna R. - DU, Yan-Jun - FAN, Ri-Dong. Sodium hexametaphosphate (SHMP)-amended calcium bentonite for slurry trench cutoff walls: workability and microstructure characteristics. In *CANADIAN GEOTECHNICAL JOURNAL*. ISSN 0008-3674, 2018, vol. 55, no. 4, pp. 528-537., Registrované v: WOS
116. [1.1] YUAN, Songhu - LIU, Xixiang - LIAO, Wenjuan - ZHANG, Peng - WANG, Xiaoming - TONG, Man. Mechanisms of electron transfer from structural Fe(II) in reduced nontronite to oxygen for production of hydroxyl radicals. In *GEOCHIMICA ET COSMOCHIMICA ACTA*. ISSN 0016-7037, 2018, vol. 223, no., pp. 422-436., Registrované v: WOS
117. [1.1] ZAVALA-FRANCO, Anai - HERNANDEZ-PATLAN, Daniel - SOLIS-CRUZ, Bruno - LOPEZ-ARELLANO, Raquel - TELLEZ-ISAIAS, Guillermo - VAZQUEZ-DURAN, Alma - MENDEZ-ALBORES, Abraham. Assessing the Aflatoxin B-1 Adsorption Capacity between Biosorbents Using an In Vitro Multicompartmental Model Simulating the Dynamic Conditions in the Gastrointestinal Tract of Poultry. In *TOXINS*. ISSN 2072-6651, 2018, vol. 10, no. 11, pp., Registrované v: WOS
118. [1.1] ZVIAGINA, Bella B. - DRITS, Victor A. - SAKHAROV, Boris A. - IVANOVSKAYA, Tatiana A. - DORZHEVA, Olga V. - MCCARTY, Douglas K. CRYSTAL-CHEMICAL REGULARITIES AND IDENTIFICATION CRITERIA IN Fe-BEARING, K-DIOCTAHEDRAL 1M MICAS FROM X-RAY DIFFRACTION AND INFRARED SPECTROSCOPY DATA. In *CLAYS AND CLAY MINERALS*. ISSN 0009-8604, 2017, vol. 65, no. 4, pp. 234-251., Registrované v: WOS

ADCA246 MADEJOVÁ, Jana - SEKERÁKOVÁ, Ľudmila - BIZOVSKÁ, Valéria - SLANÝ, Michal - JANKOVIČ, Ľuboš. Near-infrared spectroscopy as an effective tool for monitoring the conformation of alkylammonium surfactants in montmorillonite interlayers. In *Vibrational Spectroscopy*, 2016, vol. 84, p. 44-52. (2015: 1.682 - IF, Q3 - JCR, 0.592 - SJR, Q3 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0924-2031.

Citácie:

- [1.1] TSANTOS, C. - GIONIS, V. - CHRYSSIKOS, G. D. Smectite in bentonite: Near infrared systematics and estimation of layer charge. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 160, no., pp. 81-87., Registrované v: WOS

ADCA247 MADEJOVÁ, Jana - ARVAIOVÁ, Beata - KOMADEL, Peter. FTIR spectroscopic characterization of thermally treated Cu²⁺, Cd²⁺, and Li⁺ montmorillonites. In *Spectrochimica Acta A*, 1999, vol. 55, no. 12, p. 2467-2476. (1998: 0.690 - IF).

Citácie:

- [1.1] BODART, Philippe R. - DELMOTTE, L. - RIGOLET, S. - BRENDLE, J. - GOUGEON, Regis D. Li-7{F-19} TEDOR NMR to observe the lithium migration in heated montmorillonite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 157, no., pp. 204-211., Registrované v: WOS
- [1.1] MOHAMED, E. F. - AWAD, G. - ZAITAN, H. - ANDRIANTSIFERANA, C. - MANERO, M-H. Transition metals-incorporated zeolites as environmental catalysts for indoor air ozone decomposition. In *ENVIRONMENTAL TECHNOLOGY*. ISSN 0959-3330, 2018, vol. 39, no. 7, pp. 878-886., Registrované v: WOS
- [1.1] PALCHIK, N. A. - MOROZ, T. N. - MIROSHNICHENKO, L. V. Structure and Properties of Syntetic Layered Lithium-Containing Silicates. In *CRYSTALLOGRAPHY REPORTS*. ISSN 1063-7745, 2018, vol. 63, no. 7, pp. 1082-1087., Registrované v: WOS
- [1.1] REBITSKI, Ediana P. - ARANDA, Pilar - DARDER, Margarita - CARRARO, Raffaele - RUIZ-HITZKY, Eduardo. Intercalation of metformin into montmorillonite. In *DALTON TRANSACTIONS*. ISSN 1477-9226, 2018, vol. 47, no. 9, pp. 3185-

3192., Registrované v: WOS

5. [1.1] XU, Lin - LIU, Wei - CAI, Yawen - WU, Chunfang - CHEN, Lei - YANG, Shitong - WANG, Xiangke - JI, Guoxun - WANG, Shuao. Competitive sequestration of Ni(II) and Eu(III) on montmorillonite: role of molar Ni:Eu ratios and coexisting oxalate. In ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH. ISSN 0944-1344, 2018, vol. 25, no. 32, pp. 32617-32630., Registrované v: WOS

ADCA248 MADEJOVÁ, Jana - KOMADEL, Peter. Baseline studies of The Clay Minerals Society Source Clays: Infrared methods. In Clays and Clay Minerals, 2001, vol. 49, no. 5, p. 410-432. (2001 - Current Contents). ISSN 0009-8604.

Citácie:

1. [1.1] AHMED, A. - CHAKER, Y. - BELARBI, El H. - ABBAS, O. - CHOTARD, J. N. - ABASSI, H. B. - NGUYEN VAN NHIEN, A. - EL HADRI, M. - BRESSON, S. XRD and ATR/FTIR investigations of various montmorillonite clays modified by monocationic and dicationic imidazolium ionic liquids. In JOURNAL OF MOLECULAR STRUCTURE. ISSN 0022-2860, 2018, vol. 1173, no., pp. 653-664., Registrované v: WOS

2. [1.1] ALLAOUI, Assia - HATTAB, Zhour - ZERDOUM, Radia - DJELLABI, Ridha - BERREDJEM, Yamina - BESSASHIA, Wahiba - GUERFI, Kamel. Adsorption of hexavalent chromium by crushed brick: effect of operating parameters and modeling study. In DESALINATION AND WATER TREATMENT. ISSN 1944-3994, 2018, vol. 131, no., pp. 291-304., Registrované v: WOS

3. [1.1] BEJI, R. - HAMD, Wissam - KESRAOUI, A. - SEFFEN, Mongi. Effects of salts on phosphorus adsorption in alkaline Tunisian soil. In EURO-MEDITERRANEAN JOURNAL FOR ENVIRONMENTAL INTEGRATION. ISSN 2365-6433, 2017, vol. 2, no. 1, pp., Registrované v: WOS

4. [1.1] BELHOCINE, M. - HAOUI, A. - BASSOU, G. - PHOU, T. - MAURIN, D. - BANTIGNIES, J. L. - HENN, F. Isothermic heat of water adsorption and desorption in homoionic alkaline-earth montmorillonites. In CHEMICAL PHYSICS. ISSN 0301-0104, 2018, vol. 501, no., pp. 26-34., Registrované v: WOS

5. [1.1] BEN MOSHE, Shany - RYTWO, Giora. Thiamine-based organoclay for phenol removal from water. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 155, no., pp. 50-56., Registrované v: WOS

6. [1.1] BOURLIVA, A. - SIKALIDIS, A. K. - PAPADOPOULOU, L. - BETSIU, M. - MICHAILIDIS, K. - SIKALIDIS, C. - FILIPPIDIS, A. Removal of Cu²⁺ and Ni²⁺ ions from aqueous solutions by adsorption onto natural palygorskite and vermiculite. In CLAY MINERALS. ISSN 0009-8558, 2018, vol. 53, no. 1, pp. 1-15., Registrované v: WOS

7. [1.1] BUJDAKOVA, H. - BUJDAKOVA, V. - MAJEKOVA-KOSCOVA, H. - GAALOVA, B. - BIZOVSKA, V. - BOHAC, P. - BUJDAK, J. Antimicrobial activity of organoclays based on quaternary alkylammonium and alkylphosphonium surfactants and montmorillonite. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 158, no., pp. 21-28., Registrované v: WOS

8. [1.1] CELEDON, Salvador - DE CAMARGO, Andrea S. S. - FUENTEALBA, Mauricio - ARTIGAS, Vania - BENAVENTE, Eglantina - GONZALEZ, Guillermo. Highly emissive host-guest based on nanoclay intercalated with an Eu³⁺ complex bearing a new Ru²⁺ organometallic ligand. In NEW JOURNAL OF CHEMISTRY. ISSN 1144-0546, 2018, vol. 42, no. 18, pp. 15284-15294., Registrované v: WOS

9. [1.1] CHAVALI, Rama Vara Prasad - REDDY, Hari Prasad P. VOLUME CHANGE BEHAVIOR OF PHOSPHOGYPSUM TREATED CLAYEY SOILS CONTAMINATED WITH INORGANIC ACIDS A MICRO LEVEL STUDY. In JOURNAL OF ENVIRONMENTAL ENGINEERING AND LANDSCAPE MANAGEMENT. ISSN 1648-6897, 2018, vol. 26, no. 1, pp. 8-18., Registrované v: WOS

10. [1.1] CHEN, Shuling - HONG, Hanlie - HUANG, Xianyu - FANG, Qian - YIN, Ke - WANG, Chaowen - ZHANG, Yiming - CHENG, Liuling - ALGEO, Thomas J. The role of organo-clay associations in limiting organic matter decay: Insights from the Dajiuhu peat soil, central China. In GEODERMA. ISSN 0016-7061, 2018, vol. 320, no., pp. 149-160., Registrované v: WOS

11. [1.1] CHICINAS, R. Plesa - BEDELEAN, H. - STEFAN, R. - MAICANEANU, A. Ability of a montmorillonitic clay to interact with cationic and anionic dyes in aqueous solutions. In JOURNAL OF MOLECULAR STRUCTURE. ISSN 0022-2860, 2018, vol. 1154, no., pp. 187-195., Registrované v: WOS

12. [1.1] CIRAK, M. High-temperature electrocoagulation of colloidal calcareo-argillaceous suspension. In POWDER TECHNOLOGY. ISSN 0032-5910, 2018, vol. 328, no., pp. 13-25., Registrované v: WOS

13. [1.1] CISNEROS-ROSADO, D. E. - PAZ-ALPUCHE, E. F. - URIBE-CALDERON, J. A. The Effect of Surface Modification of Palygorskite on the Morphology, Mechanical, and Thermal Properties of Nylon 6/Palygorskite Nanocomposites Prepared by Melt Compounding. In POLYMER COMPOSITES. ISSN 0272-8397, 2018, vol. 39, no., pp. E1531-E1543., Registrované v: WOS

14. [1.1] DANNER, Tobias - NORDEN, Geir - JUSTNES, Harald. Characterisation of calcined raw clays suitable as supplementary cementitious materials. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 162, no., pp. 391-402., Registrované v: WOS

15. [1.1] DAO, Kalifala - OUEDRAOGO, Moussa - MILLOGO, Younoussa - AUBERT, Jean-Emmanuel - GOMINA, Moussa. Thermal, hydric and mechanical behaviours of adobes stabilized with cement. In CONSTRUCTION AND BUILDING MATERIALS. ISSN 0950-0618, 2018, vol. 158, no., pp. 84-96., Registrované v: WOS

16. [1.1] DOS SANTOS, E. C. - GATES, W. P. - MICHELS, L. - JURANYI, F. - MIKKELSEN, A. - DA SILVA, G. J. - FOSSUM, J. O. - BORDALLO, H. N. The pH influence on the intercalation of the bioactive agent ciprofloxacin in fluorohectorite. In APPLIED CLAY SCIENCE. ISSN 0169-1317, 2018, vol. 166, no., pp. 288-298., Registrované v: WOS

17. [1.1] EHLMANN, Bethany L. - HODYSS, Robert - BRISTOW, Thomas F. - ROSSMAN, George R. - AMMANNITO, Eleonora - DE SANCTIS, M. Cristina - RAYMOND, Carol A. Ambient and cold-temperature infrared spectra and XRD patterns of ammoniated phyllosilicates and carbonaceous chondrite meteorites relevant to Ceres and other solar system bodies. In METEORITICS & PLANETARY SCIENCE. ISSN 1086-9379, 2018, vol. 53, no. 9, pp. 1884-1901., Registrované v: WOS

18. [1.1] FERNANDEZ, Raul - GONZALEZ-SANTAMARIA, Daniel - ANGULO, Maria - TORRES, Elena - ISABEL RUIZ, Ana - JESUS TURRERO, Maria - CUEVAS, Jaime. Geochemical conditions for the formation of Mg silicates phases in bentonite and implications for radioactive waste disposal. In APPLIED GEOCHEMISTRY. ISSN 0883-2927, 2018, vol. 93, no., pp. 1-9., Registrované v: WOS

19. [1.1] FERNANDEZ, Raul - ISABEL RUIZ, Ana - GARCIA-DELGADO, Carlos - ENRIQUE GONZALEZ-SANTAMARIA, Daniel - ANTON-HERRERO, Rafael - YUNTA, Felipe - POYO, Caudia - HERNANDEZ, Andrea - EYMAR, Enrique - CUEVAS, Jaime. Stevensite-based geofilter for the retention of tetracycline from water. In SCIENCE OF THE TOTAL ENVIRONMENT.

ISSN 0048-9697, 2018, vol. 645, no., pp. 146-155., Registrované v: WOS

20. [1.1] FISCHER, P. - POETHIG, R. - GUCKER, B. - VENOHR, M. Phosphorus saturation and superficial fertilizer application as key parameters to assess the risk of diffuse phosphorus losses from agricultural soils in Brazil. In *SCIENCE OF THE TOTAL ENVIRONMENT*. ISSN 0048-9697, 2018, vol. 630, no., pp. 1515-1527., Registrované v: WOS

21. [1.1] GAL, Agnes - IONESCU, Corina - BAJUSZ, Matyas - CODREA, Vlad A. - HOECK, Volker - BARBU-TUDORAN, Lucian - SIMON, Viorica - MURESAN-POP, Marieta - CSOK, Zsolt. Composition, technology and provenance of Roman pottery from Napoca (Cluj-Napoca, Romania). In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 4, pp. 621-641., Registrované v: WOS

22. [1.1] GOMEZ, C. - COULOUMA, G. Importance of the spatial extent for using soil properties estimated by laboratory VNIR/SWIR spectroscopy: Examples of the clay and calcium carbonate content. In *GEODERMA*. ISSN 0016-7061, 2018, vol. 330, no., pp. 244-253., Registrované v: WOS

23. [1.1] GYOLLAI, Ildiko - POLGARI, Marta - BIRO, Lorant - VIGH, Tamas - KOVACS, Tibor - PAL-MOLNAR, Elemer. FOSSILIZED BIOMATS AS THE POSSIBLE SOURCE OF HIGH NATURAL RADIONUCLIDE CONTENT AT THE JURASSIC URKUT MANGANESE ORE DEPOSIT, HUNGARY. In *CARPATHIAN JOURNAL OF EARTH AND ENVIRONMENTAL SCIENCES*. ISSN 1842-4090, 2018, vol. 13, no. 2, pp. 477-487., Registrované v: WOS

24. [1.1] HAHN, Annette - VOGEL, Hendrik - ANDO, Sergio - GARZANTI, Eduardo - KUHN, Gerhard - LANTZSCH, Hendrik - SCHUEUERMANN, Jan - VOGT, Christoph - ZABEL, Matthias. Using Fourier transform infrared spectroscopy to determine mineral phases in sediments. In *SEDIMENTARY GEOLOGY*. ISSN 0037-0738, 2018, vol. 375, no., pp. 27-35., Registrované v: WOS

25. [1.1] HONG, Lei - ROMANOV, Vyacheslav. Experimental Studies: Molecular Interactions at Clay Interfaces. In *GREENHOUSE GASES AND CLAY MINERALS: ENLIGHTENING DOWN-TO-EARTH ROAD MAP TO BASIC SCIENCE OF CLAY-GREENHOUSE GAS INTERFACES*. ISSN 1865-3529, 2018, vol., no., pp. 95-123., Registrované v: WOS

26. [1.1] HORN, Karen R. Time takes its toll: Detection of organic binder media in ochre paints with visible near-infrared and short-wave infrared reflectance spectroscopy. In *JOURNAL OF ARCHAEOLOGICAL SCIENCE-REPORTS*. ISSN 2352-409X, 2018, vol. 21, no., pp. 10-20., Registrované v: WOS

27. [1.1] IANNUCELLI, Valentina - MARETTI, Eleonora - BELLINI, Alessia - Malferrari, Daniele - ORI, Guido - MONTORSI, Monia - BONDI, Moreno - TRUZZI, Eleonora - LEO, Eliana. Organo-modified bentonite for gentamicin topical application: Interlayer structure and in vivo skin permeation. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 158, no., pp. 158-168., Registrované v: WOS

28. [1.1] KASPRZHITSKII, Anton - LAZORENKO, Georgy - KHATER, Antoine - YAVNA, Victor. Mid-Infrared Spectroscopic Assessment of Plasticity Characteristics of Clay Soils. In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 5, pp., Registrované v: WOS

29. [1.1] KERESZTURI, Akos - FINTOR, Krisztian - GYOLLAI, Ildiko - KERESZTY, Zsolt - SZABO, Mate - SZALAI, Zoltan - WALTER, Ena. Shock heterogeneity and shock history of the recently found ordinary Csatalja chondrite in Hungary. In *GEOLOGICAL QUARTERLY*. ISSN 1641-7291, 2018, vol. 62, no. 2, pp. 433-446., Registrované v: WOS

30. [1.1] KHOSRAVI, Vahid - ARDEJANI, Faramarz Doulati - YOUSEFI, Saeed - ARYAFAR, Ahmad. Monitoring soil lead and zinc contents via combination of spectroscopy with extreme learning machine and other data mining methods. In *GEODERMA*. ISSN 0016-7061, 2018, vol. 318, no., pp. 29-41., Registrované v: WOS

31. [1.1] LAZORENKO, Georgy - KASPRZHITSKII, Anton - YAVNA, Victor. Synthesis and structural characterization of betaine- and imidazoline-based organoclays. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 692, no., pp. 264-270., Registrované v: WOS

32. [1.1] LEMMA, Roxana - CASTELLANO, Cristina C. - BONAVETTI, Viviana L. - TREZZA, Monica A. - RAHHAL, Viviana F. - IRASSAR, Edgardo F. Thermal Transformation of Illitic-Chlorite Clay and Its Pozzolanic Activity. In *CALCINED CLAYS FOR SUSTAINABLE CONCRETE*. ISSN 2211-0844, 2018, vol. 16, no., pp. 266-272., Registrované v: WOS

33. [1.1] LI, Zhaohui - POTTER, Nicholas - RASMUSSEN, Joseph - WENG, Jianle - LV, Guocheng. Removal of rhodamine 6G with different types of clay minerals. In *CHEMOSPHERE*. ISSN 0045-6535, 2018, vol. 202, no., pp. 127-135., Registrované v: WOS

34. [1.1] LIAO, Yuanyuan - PICOT, Pierre - BRUBACH, Jean-Blaise - ROY, Pascale - LE CAER, Sophie - THILL, Antoine. Self-supporting thin films of imogolite and imogolite-like nanotubes for infrared spectroscopy. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 164, no., pp. 58-67., Registrované v: WOS

35. [1.1] LOZANO-MORALES, Virginia - GARDI, Ido - NIR, Shlomo - UNDABEYTIA, Tomas. Removal of pharmaceuticals from water by clay-cationic starch sorbents. In *JOURNAL OF CLEANER PRODUCTION*. ISSN 0959-6526, 2018, vol. 190, no., pp. 703-711., Registrované v: WOS

36. [1.1] MARSH, A. - HEATH, A. - PATUREAU, P. - EVERNDEN, M. - WALKER, P. A mild conditions synthesis route to produce hydrosodalite from kaolinite, compatible with extrusion processing. In *MICROPOROUS AND MESOPOROUS MATERIALS*. ISSN 1387-1811, 2018, vol. 264, no., pp. 125-132., Registrované v: WOS

37. [1.1] MROCZKOWSKA-SZERSZEN, Maja - ORZECZOWSKI, Mateusz. Infrared spectroscopy methods in reservoir rocks analysis-semiquantitative approach for carbonate rocks. In *NAFTA-GAZ*. ISSN 0867-8871, 2018, vol. 74, no. 11, pp. 802-812., Registrované v: WOS

38. [1.1] MUHAMMAD, Nurmunira - SIDDIQUA, Sumi - LATIFI, Nima. Solidification of Subgrade Materials Using Magnesium Alkalinization: A Sustainable Additive for Construction. In *JOURNAL OF MATERIALS IN CIVIL ENGINEERING*. ISSN 0899-1561, 2018, vol. 30, no. 10, pp., Registrované v: WOS

39. [1.1] MUTHU, Jacob - PRISCILLA, Janet - ODESHI, Akindele - KUPPEN, Nalen. Characterisation of coir fibre hybrid composites reinforced with clay particles and glass spheres. In *JOURNAL OF COMPOSITE MATERIALS*. ISSN 0021-9983, 2018, vol. 52, no. 5, pp. 593-607., Registrované v: WOS

40. [1.1] NEGREANU, Stefan - SOARE, Barbara - AVRAM, Sorin. CLAY MINERALS IDENTIFIED IN RED QUATERNARY DEPOSITS, FROM VALEA ANILOR AREA (MEHEDINTI COUNTY, ROMANIA), USING XRD AND IR ABSORPTION ANALYSIS. In *CARPATHIAN JOURNAL OF EARTH AND ENVIRONMENTAL SCIENCES*. ISSN 1842-4090, 2018, vol. 13, no. 2, pp. 447-452., Registrované v: WOS

41. [1.1] NGNIE, Gaelle - BAITAN, Daniela - DEDZO, Gustave Kenne - DETELLIER, Christian. Sedimentation of fine particles of kaolinite and polymer-coated kaolinite in cyclohexane: Implications for fines removal from extracted bitumen in non-aqueous processes. In *FUEL*. ISSN 0016-2361, 2018, vol. 234, no., pp. 218-224., Registrované v: WOS
42. [1.1] OYEBANJO, O. M. - EKOSSE, G. E. - ODIYO, J. O. Mineral Constituents and Kaolinite Crystallinity of the < 2 µm Fraction of Cretaceous-Paleogene/Neogene Kaolins from Eastern Dahomey and Niger Delta Basins, Nigeria. In *OPEN GEOSCIENCES*. ISSN 2391-5447, 2018, vol. 10, no. 1, pp. 157-166., Registrované v: WOS
43. [1.1] PAJARITO, Bryan B. - CASTANEDA, Kayla C. - JERESANO, Sofia Denise M. - REPOQUIT, Dominique Ann N. Reduction of Offensive Odor from Natural Rubber Using Zinc-Modified Bentonite. In *ADVANCES IN MATERIALS SCIENCE AND ENGINEERING*. ISSN 1687-8434, 2018, vol., no., pp., Registrované v: WOS
44. [1.1] PAVLINAKOVA, Veronika - FOHLEROVA, Zdenka - PAVLINAK, David - KHUNOVA, Viera - VOJTOVA, Lucy. Effect of halloysite nanotube structure on physical, chemical, structural and biological properties of elastic polycaprolactone/gelatin nanofibers for wound healing applications. In *MATERIALS SCIENCE & ENGINEERING C-MATERIALS FOR BIOLOGICAL APPLICATIONS*. ISSN 0928-4931, 2018, vol. 91, no., pp. 94-102., Registrované v: WOS
45. [1.1] PELAYO, M. - MARCO, J. F. - FERNANDEZ, A. M. - VERGARA, L. - MELON, A. M. - PEREZ DEL VILLAR, L. Infrared and Mossbauer spectroscopy of Fe-rich smectites from Morron de Mateo bentonite deposit (Spain). In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 1, pp. 17-28., Registrované v: WOS
46. [1.1] PEROVSKIY, Igor A. - KHRAMENKOVA, Elena V. - PIDKO, Evgeny A. - KRIVOSHAPKIN, Pavel V. - VINOGRADOV, Alexandr V. - KRIVOSHAPKINA, Elena F. Efficient extraction of multivalent cations from aqueous solutions into sitinakite-based sorbents. In *CHEMICAL ENGINEERING JOURNAL*. ISSN 1385-8947, 2018, vol. 354, no., pp. 727-739., Registrované v: WOS
47. [1.1] PEYNE, Julie - GHARZOUNI, Ameni - SOBRADOS, Isabel - ROSSIGNOL, Sylvie. Identifying the differences between clays used in the brick industry by various methods: Iron extraction and NMR spectroscopy. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 160, no., pp. 290-298., Registrované v: WOS
48. [1.1] POZO-ANTONIO, J. S. - RIVAS, T. - CARRERA, F. - GARCIA, L. Deterioration processes affecting prehistoric rock art engravings in granite in NW Spain. In *EARTH SURFACE PROCESSES AND LANDFORMS*. ISSN 0197-9337, 2018, vol. 43, no. 11, pp. 2435-2448., Registrované v: WOS
49. [1.1] REN, Li-ying - HONG, Zhi-neng - LIU, Zhao-dong - XU, Ren-kou. ATR-FTIR investigation of mechanisms of *Bacillus subtilis* adhesion onto variable- and constant-charge soil colloids. In *COLLOIDS AND SURFACES B-BIOINTERFACES*. ISSN 0927-7765, 2018, vol. 162, no., pp. 288-295., Registrované v: WOS
50. [1.1] REZAEI, R. - MASSINAEI, M. - MOGHADDAM, A. Zeraatkar. Removal of the residual xanthate from flotation plant tailings using modified bentonite. In *MINERALS ENGINEERING*. ISSN 0892-6875, 2018, vol. 119, no., pp. 1-10., Registrované v: WOS
51. [1.1] RITZ, Michal - VALASKOVA, Marta. Infrared and Raman spectroscopy of three commercial vermiculites doped with cerium dioxide nanoparticles. In *SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY*. ISSN 1386-1425, 2018, vol. 201, no., pp. 39-45., Registrované v: WOS
52. [1.1] SHARMA, L. K. - SIRDESAI, N. N. - SHARMA, K. M. - SINGH, T. N. Experimental study to examine the independent roles of lime and cement on the stabilization of a mountain soil: A comparative study. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 152, no., pp. 183-195., Registrované v: WOS
53. [1.1] SILVA, Gustavo Thalmer M. - SILVA, Cassio P. - GEHLEN, Marcelo H. - OAKE, Jessy - BOHNE, Cornelia - QUINA, Frank H. Organic/inorganic hybrid pigments from flavylum cations and palygorskite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 162, no., pp. 478-486., Registrované v: WOS
54. [1.1] SILVA-VALENZUELA, Maria das Gracas - CHAMBI-PERALTA, Marvin Marco - SAYEG, Isaac Jamil - DE SOUZA CARVALHO, Flavio Machado - WANG, Shu Hui - VALENZUELA-DIAZ, Francisco Rolando. Enrichment of clay from Vitoria da Conquista (Brazil) for applications in cosmetics. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 155, no., pp. 111-119., Registrované v: WOS
55. [1.1] SOMELAR, Peeter - VAHUR, Signe - HAMILTON, Tark S. - MAHANEY, William C. - BARENDREGT, Rene W. - COSTA, Pedro. Sand coatings in paleosols: Evidence of weathering across the Plio-Pleistocene boundary to modern times on Mt. Kenya. In *GEOMORPHOLOGY*. ISSN 0169-555X, 2018, vol. 317, no., pp. 91-106., Registrované v: WOS
56. [1.1] SONG, Yinxian - LI, Jizhou - MAO, Changping - LI, Tianyuan - FENG, Yuexing. THE ESTIMATION OF HEAVY METALS IN RIVERS SEDIMENTS IN CHANGJIANG RIVER DELTA BY VISIBLE/NEAR INFRARED (VIS/NIR) SPECTROSCOPY. In *FRESENIUS ENVIRONMENTAL BULLETIN*. ISSN 1018-4619, 2018, vol. 27, no. 9, pp. 6184-6194., Registrované v: WOS
57. [1.1] SRIVASTAVA, Priyeshu - SIDDIAH, N. Siva - SANGODE, S. J. - MESHRAM, D. C. Mineralogy and geochemistry of various colored boles from the Deccan volcanic province: Implications for paleoweathering and paleoenvironmental conditions. In *CATENA*. ISSN 0341-8162, 2018, vol. 167, no., pp. 44-59., Registrované v: WOS
58. [1.1] STAWINSKI, Wojciech - WEGRZYN, Agnieszka - MORDARSKI, Grzegorz - SKIBA, Michal - FREITAS, Olga - FIGUEIREDO, Sonia. Sustainable adsorbents formed from by-product of acid activation of vermiculite and leached-vermiculite-LDH hybrids for removal of industrial dyes and metal cations. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 161, no., pp. 6-14., Registrované v: WOS
59. [1.1] STEMPFLE, Sabrina - LINSTAEDTER, Joerg - NICKEL, Klaus G. - MIKDDAD, Abdeslam - SCHMIDT, Patrick. Early Neolithic pottery of Ifri n'Etsedda, NE-Morocco Raw materials and fabrication techniques. In *JOURNAL OF ARCHAEOLOGICAL SCIENCE-REPORTS*. ISSN 2352-409X, 2018, vol. 19, no., pp. 200-212., Registrované v: WOS
60. [1.1] TONG, Dongshen - WAN, Min - ZHENG, Youmiao - HAN, Yanrui - HU, Jun. Polyaspartic acid-grafted montmorillonite composite: a new adsorbent for the removal of copper(II), zinc(II), nickel(II). In *DESALINATION AND WATER TREATMENT*. ISSN 1944-3994, 2018, vol. 133, no., pp. 103-113., Registrované v: WOS
61. [1.1] VARMA, Atul Kumar - MISHRA, Divya Kumari - SAMAD, Suresh Kumar - PRASAD, Amal Kishore - PANIGRAHI, Durga Charan - MENDHE, Vinod Atmaram - SINGH, Bhagwan D. Geochemical and organo-petrographic characterization for hydrocarbon generation from Barakar Formation in Auranga Basin, India. In *INTERNATIONAL JOURNAL OF COAL GEOLOGY*. ISSN 0166-5162, 2018, vol. 186, no., pp. 97-114., Registrované v: WOS
62. [1.1] VLCEK, Vitezslav - POSPISILOVA, Lubica - UHLIK, Peter. Mineralogy and Chemical Composition of Cryosols and Andosols in Antarctica. In *SOIL AND WATER RESEARCH*. ISSN 1801-5395, 2018, vol. 13, no. 2, pp. 61-73., Registrované v: WOS
63. [1.1] WANNER, Christoph - POETHIG, Rosemarie - CARRERO, Sergio - FERNANDEZ-MARTINEZ, Alejandro - JAEGER,

Christian - FURRER, Gerhard. Natural occurrence of nanocrystalline Al-hydroxysulfates: Insights on formation, Al solubility control and As retention. In *GEOCHIMICA ET COSMOCHIMICA ACTA*. ISSN 0016-7037, 2018, vol. 238, no., pp. 252-269., Registrované v: WOS

64. [1.1] WĘGRZYŃ, Agnieszka - STAWINSKI, Wojciech - FREITAS, Olga - KOMEDERA, Kamila - BLACHOWSKI, Artur - JECZMIONEK, Lukasz - DANKO, Tomasz - MORDARSKI, Grzegorz - FIGUEIREDO, Sonia. Study of adsorptive materials obtained by wet fine milling and acid activation of vermiculite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 155, no., pp. 37-49., Registrované v: WOS

65. [1.1] WIHEEB, A. D. - SHAKIR, S. W. - OTHMAN, M. R. Synthesis and Characterization of Mesoporous Hydrotalcite-Alumina Membrane for Carbon Dioxide Enrichment. In *INTERNATIONAL CONFERENCE ON MATERIALS ENGINEERING AND SCIENCE*. ISSN 1757-8981, 2018, vol. 454, no., pp., Registrované v: WOS

66. [1.1] YANG, Min - YE, Meifang - HAN, Haihui - REN, Guangli - HAN, Ling - ZHANG, Zhuan. Near-Infrared Spectroscopic Study of Chlorite Minerals. In *JOURNAL OF SPECTROSCOPY*. ISSN 2314-4920, 2018, vol., no., pp., Registrované v: WOS

67. [1.1] ZHANG, Zhi F. - WANG, Wen B. - MU, B. - WANG, Ai Q. THIOUREA-INDUCED CHANGE OF STRUCTURE AND COLOR OF BRICK-RED Palygorskite. In *CLAYS AND CLAY MINERALS*. ISSN 0009-8604, 2018, vol. 66, no. 5, pp. 403-414., Registrované v: WOS

ADCA249 MADEJOVÁ, Jana - JANEK, Marián - KOMADEL, Peter - HERBERT, H.-J. - MOOG, H.C. FTIR analyses of water in MX-80 bentonite compacted from high salinary salt solution systems. In *Applied Clay Science*, 2002, vol. 20, no. 6, p. 255-271.

Citácie:

1. [1.1] BELHOCINE, M. - HAOUI, A. - BASSOU, G. - PHOU, T. - MAURIN, D. - BANTIGNIES, J. L. - HENN, F. Isothermic heat of water adsorption and desorption in homoionic alkaline-earth montmorillonites. In *CHEMICAL PHYSICS*. ISSN 0301-0104, 2018, vol. 501, no., pp. 26-34., Registrované v: WOS

2. [1.1] GHARZOUNI, A. - OUAMARA, L. - SOBRADOS, I. - ROSSIGNOL, S. Alkali-activated materials from different aluminosilicate sources: Effect of aluminum and calcium availability. In *JOURNAL OF NON-CRYSTALLINE SOLIDS*. ISSN 0022-3093, 2018, vol. 484, no., pp. 14-25., Registrované v: WOS

3. [1.1] IANNUCELLI, Valentina - MARETTI, Eleonora - BELLINI, Alessia - Malferrari, Daniele - ORI, Guido - MONTORSI, Monia - BONDI, Moreno - TRUZZI, Eleonora - LEO, Eliana. Organo-modified bentonite for gentamicin topical application: Interlayer structure and in vivo skin permeation. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 158, no., pp. 158-168., Registrované v: WOS

4. [1.1] JOHNSTON, Cliff T. Clay mineral-water interactions. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS*, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 89-124., Registrované v: WOS

5. [1.1] KOMNITSAS, Kostas - PETRAKIS, Evangelos - PANTELAKI, Olga - KRITIKAKI, Anna. Column Leaching of Greek Low-Grade Limonitic Laterites. In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 9, pp., Registrované v: WOS

6. [1.1] LI, Aobo - ZHAO, Xiaoguang - ANDERSON, Stephan - ZHANG, Xin. Silica Nanowire Growth on *Coscinodiscus* Species Diatom Frustules via Vapor-Liquid-Solid Process. In *SMALL*. ISSN 1613-6810, 2018, vol. 14, no. 47, pp., Registrované v: WOS

7. [1.1] NDZANA, Georges Martial - HUANG, Li - WANG, Jin Bo - ZHANG, Zhi Yi. Characteristics of clay minerals in soil particles from an argillic horizon of Alfisol in central China. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 151, no., pp. 148-156., Registrované v: WOS

8. [1.1] SHEN, Wei - LI, Lin - ZHOU, Huijun - ZHOU, Qing - CHEN, Meng - ZHU, Jianxi. Effects of charge density on the hydration of siloxane surface of montmorillonite: A molecular dynamics simulation study. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 159, no., pp. 10-15., Registrované v: WOS

ADCA250 MADEJOVÁ, Jana - JANKOVIČ, Ľuboš - PENTRÁK, Martin - KOMADEL, Peter. Benefits of near-infrared spectroscopy for characterization of selected organo-montmorillonites. In *Vibrational Spectroscopy*, 2011, vol. 57, no. 1, p. 8-14. (2010: 2.083 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0924-2031.

Citácie:

1. [1.1] Jlassi, Khoulood - ABIDI, Rym - BENNA, Memia - CHEHIMI, Mohamed M. - KASAK, Peter - KRUPA, Igor. Bentonite-decorated calix [4] arene: A new, promising hybrid material for heavy-metal removal. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 161, no., pp. 15-22., Registrované v: WOS

2. [1.2] SIREGAR, Sri Hilma - WIJAYA, Karna - KUNARTI, Eko Sri - SYOUFIAN, Akhmad - SUYANTA. Preparation and characterization of montmorillonite-cetyl trimethylammonium bromide. In *Asian Journal of Chemistry*. ISSN 09707077, 2018-01-01, 30, 1, pp. 25-28., Registrované v: SCOPUS

ADCA251 MADEJOVÁ, Jana - KEČKÉŠ, Jozef - PÁLKOVÁ, Helena - KOMADEL, Peter. Identification of components in smectite/kaolinite mixtures. In *Clay Minerals*, 2002, vol. 37, no. 2, p. 377-388. (2001: 0.610 - IF, karentované - CCC). (2002 - Current Contents). ISSN 0009-8558.

Citácie:

1. [1.1] AL-ESSA, Khansaa. NaCl Activated Jordanian Bentonite for Olive Mill Waste water Treatment: Evaluation of Physicochemical Properties, Adsorption of Phenolic Compounds: Isotherms and Thermodynamic Studies. In *RESEARCH JOURNAL OF PHARMACEUTICAL BIOLOGICAL AND CHEMICAL SCIENCES*. ISSN 0975-8585, 2018, vol. 9, no. 3, pp. 1362-1384., Registrované v: WOS

2. [1.1] BEN SALAH, Imed - SDIRI, Ali - JEMAI, Mouda Ben M';barek - BOUGHDIRI, Mabrouk. Potential use of the lower cretaceous clay (Kef area, Northwestern Tunisia) as raw material to supply ceramic industry. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 161, no., pp. 151-162., Registrované v: WOS

3. [1.1] BISHOP, Janice L. Remote Detection of Phyllosilicates on Mars and Implications for Climate and Habitability. In *FROM HABITABILITY TO LIFE ON MARS*, 2018, vol., no., pp. 37-75., Registrované v: WOS

4. [1.1] FAN, Ruqin - YANG, Xueming - DRURY, Craig F. - ZHANG, Zhenhua. Curve-fitting techniques improve the mid-infrared analysis of soil organic carbon: a case study for Brookston clay loam particle-size fractions. In *SCIENTIFIC REPORTS*. ISSN 2045-2322, 2018, vol. 8, no., pp., Registrované v: WOS

- ADCA252 MACHÁČEK, Jan - GEDEON, Ondrej - LIŠKA, Marek - MARHOUL, Filip. Molecular simulations of silicate melts doped with sulphur and nitrogen. In *Journal of Non-Crystalline Solids*, 2010, vol. 356, no. 44-49, p. 2458-2464. (2009: 1.252 - IF, karentované - CCC). (2010 - Current Contents, SCOPUS). ISSN 0022-3093.
Citácie:
1. [1.1] LIERENFELD, Matthias Bernhard - ZAJACZ, Zoltan - BACHMANN, Olivier - ULMER, Peter. Sulfur diffusion in dacitic melt at various oxidation states: Implications for volcanic degassing. In *GEOCHIMICA ET COSMOCHIMICA ACTA*. ISSN 0016-7037, 2018, vol. 226, no., pp. 50-68., Registrované v: WOS
- ADCA253 MACHÁČEK, Jan - KOSTKA, Petr - LIŠKA, Marek - ZAVADIL, Jiří - GEDEON, Ondrej. Calculation and analysis of vibrational spectra of PbCl₂-Sb₂O₃-TeO₂ glass from first principles. In *Journal of Non-Crystalline Solids*, 2011, vol. 357, no. 14, p. 2562-2570. (2010: 1.492 - IF, karentované - CCC). (2011 - Current Contents, SCOPUS). ISSN 0022-3093.
Citácie:
1. [1.1] CASTRO, Alexandre - BREHAULT, Antoine - CARCREFF, Julie - BOSAK, Ondrej - KUBLIHA, Marian - TRNOVCOVA, Viera - DOMANKOVA, Maria - SILJEGOVIC, Mirjana - CALVEZ, Laurent - LABAS, Vladimir - LE COQ, David. Lithium and lead chloride antimonate glasses. In *JOURNAL OF NON-CRYSTALLINE SOLIDS*. ISSN 0022-3093, 2018, vol. 499, no., pp. 66-74., Registrované v: WOS
- ADCA254 MACHÁČEK, Jan - GEDEON, Ondrej - LIŠKA, Marek. Group connectivity in binary silicate glasses. In *Journal of Non-Crystalline Solids*, 2006, vol. 352, no. 21-22, p. 2173-2179. (2005: 1.264 - IF, karentované - CCC). (2006 - Current Contents, SCOPUS). ISSN 0022-3093.
Citácie:
1. [1.1] JARDON-ALVAREZ, Daniel - SANDERS, Kevin J. - PHYO, Pyae - BALTISBERGER, Jay H. - GRANDINETTI, Philip J. Cluster formation of network-modifier cations in cesium silicate glasses. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 9, pp., Registrované v: WOS
2. [1.1] SHEKHOVTSOVA, J. - ZHERNOVSKY, I. - KOVTUN, M. - KOZHUKHOVA, N. - ZHERNOVSKAYA, I. - KEARSLEY, E. Estimation of fly ash reactivity for use in alkali-activated cements A step towards sustainable building material and waste utilization. In *JOURNAL OF CLEANER PRODUCTION*. ISSN 0959-6526, 2018, vol. 178, no., pp. 22-33., Registrované v: WOS
- ADCA255 MALKINA, Oľga - KOMOROVSKÝ, Stanislav - VISSCHER, Lucas - MALKIN, Vladimír. Note: Counterintuitive gauge-dependence of nuclear magnetic resonance shieldings for rare-gas dimers: Does a natural gauge-origin for spherical atoms exist? In *Journal of Chemical Physics*, 2011, vol. 134, no. 8, p. 086101-1-086101-2. (2010: 2.921 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0021-9606.
Citácie:
1. [1.1] GLASBRENNER, Michael - VOGLER, Sigurd - OCHSENFELD, Christian. Gauge-origin dependence in electronic g-tensor calculations. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 21, pp., Registrované v: WOS
- ADCA256 MALKINA, Oľga - KŘÍSTKOVÁ, Anežka - MALKIN, Elena - KOMOROVSKÝ, Stanislav - MALKIN, Vladimír. Illumination of the effect of the overlap of lone-pairs on indirect nuclear spin-spin coupling constants. In *Physical Chemistry Chemical Physics*, 2011, vol. 13, no. 35, p. 16015-16021. (2010: 3.453 - IF, karentované - CCC). (2011 - Current Contents). ISSN 1463-9076.
Citácie:
1. [1.1] SHENDEROVICH, Ilya G. Simplified calculation approaches designed to reproduce the geometry of hydrogen bonds in molecular complexes in aprotic solvents. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 12, pp., Registrované v: WOS
- ADCA257 MALKINA, Oľga - MALKIN, Vladimír. Visualization of nuclear spin-spin coupling pathways by real-space functions. In *Angewandte Chemie*, 2003, vol. 42, no. 36, p. 4335-4338. ISSN 1433-7851.
Citácie:
1. [1.1] SIEHL, Hans-Ullrich. The Conundrum of the (C₄H₇)(+) Cation: Bicyclobutonium and Related Carbocations. In *ADVANCES IN PHYSICAL ORGANIC CHEMISTRY, VOL 52*. ISSN 0065-3160, 2018, vol. 52, no., pp. 1-47., Registrované v: WOS
- ADCA258 MALKINA, Oľga - VAARA, Juha - SCHIMMELPFENNIG, Bernd - MUNZAROVÁ, Markéta - MALKIN, Vladimír - KAUPP, Martin. Density functional calculations of electronic g-tensors using spin-orbit pseudopotentials and mean-field all-electron spin-orbit operators. In *Journal of the American Chemical Society*, 2000, vol. 122, no. 38, p. 9206-9218. ISSN 0002-7863.
Citácie:
1. [1.1] GLASBRENNER, Michael - VOGLER, Sigurd - OCHSENFELD, Christian. Gauge-origin dependence in electronic g-tensor calculations. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 21, pp., Registrované v: WOS
2. [1.1] SAITOW, Masaaki - NEESE, Frank. Accurate spin-densities based on the domain-based local pair-natural orbital coupled-cluster theory. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 3, pp., Registrované v: WOS
3. [1.1] SAYFUTYAROVA, Elvira R. - CHAN, Garnet Kin-Lic. Electron paramagnetic resonance g-tensors from state interaction spin-orbit coupling density matrix renormalization group. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 18, pp., Registrované v: WOS
- ADCA259 MALKINA, Oľga - SCHIMMELPFENNIG, Bernd - KAUPP, Martin - HESS, B.A. - CHANDRA, P. - WAHLGREN, U. - MALKIN, Vladimír. Spin-orbit corrections to NMR shielding constants from density functional theory. How important are the two-electron terms? In *Chemical Physics Letters*, 1998, vol. 296, no. 1-2, p. 93-104. (1997: 2.440 - IF, karentované - CCC). (1998 - Current Contents).

Citácie:

1. [1.1] AUCAR, Gustavo A. - MELO, Juan I. - AGUSTIN AUCAR, Ignacio - MALDONADO, Alejandro F. Foundations of the LRESC model for response properties and some applications. In *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY*. ISSN 0020-7608, 2018, vol. 118, no. 1, pp., Registrované v: WOS
2. [1.1] RUSAKOV, Yu. Yu. - RUSAKOVA, I. L. Relativistic heavy atom effect on C-13 NMR chemical shifts initiated by adjacent multiple chalcogens. In *MAGNETIC RESONANCE IN CHEMISTRY*. ISSN 0749-1581, 2018, vol. 56, no. 8, pp. 716-726., Registrované v: WOS
3. [1.1] RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic effects in the NMR spectra of compounds containing heavy chalcogens. In *MENDELEEV COMMUNICATIONS*. ISSN 0959-9436, 2018, vol. 28, no. 1, pp. 1-13., Registrované v: WOS

ADCA260 MALKINA, Oľga - SALAHUB, Dennis R. - MALKIN, Vladimír. Nuclear magnetic resonance spin-spin coupling constants from density functional theory: Problems and results. In *Journal of Chemical Physics*, 1996, vol. 105, no. 19, p. 8793-8800. (1995: 3.610 - IF, karentované - CCC). (1996 - Current Contents, WOS, SCOPUS). ISSN 0021-9606.

Citácie:

1. [1.1] ADAMSON, Jasper - NAZARSKI, Ryszard B. - JARVET, Juri - PEHK, Tonis - AAV, Riina. Shortfall of B3LYP in Reproducing NMR J(CH) Couplings in Some Isomeric Epoxy Structures with Strong Stereoelectronic Effects: A Benchmark Study on DFT Functionals. In *CHEMPHYSICHEM*. ISSN 1439-4235, 2018, vol. 19, no. 5, pp. 631-642., Registrované v: WOS

ADCA261 MALKIN, Elena - REPISKÝ, Michal - KOMOROVSKÝ, Stanislav - MACH, Pavel - MALKINA, Oľga - MALKIN, Vladimír. Effects of finite size nuclei in relativistic four-component calculations of hyperfine structure. In *Journal of Chemical Physics*, 2011, vol. 134, no. 4, p. 044111-1-044111-8. (2010: 2.921 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] AGUSTIN AUCAR, I. - GIMENEZ, Carlos A. - AUCAR, Gustavo A. Influence of the nuclear charge distribution and electron correlation effects on magnetic shieldings and spin-rotation tensors of linear molecules. In *RSC ADVANCES*. ISSN 2046-2069, 2018, vol. 8, no. 36, pp. 20234-20249., Registrované v: WOS
2. [1.1] FERNANDEZ, Estefania - MORENO-GONZALEZ, Marta - MOLINER, Manuel - BLASCO, Teresa - BORONAT, Mercedes - CORMA, Avelino. Modeling of EPR Parameters for Cu(II): Application to the Selective Reduction of NO_x Catalyzed by Cu-Zeolites. In *TOPICS IN CATALYSIS*. ISSN 1022-5528, 2018, vol. 61, no. 9-11, pp. 810-832., Registrované v: WOS
3. [1.1] SCHATTENBERG, Caspar J. - MAIER, Toni M. - KAUPP, Martin. Lessons from the Spin-Polarization/Spin-Contamination Dilemma of Transition-Metal Hyperfine Couplings for the Construction of Exchange-Correlation Functionals. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 11, pp. 5653-5672., Registrované v: WOS

ADCA262 MALKIN, Elena - MALKIN, Irina - MALKINA, Oľga - MALKIN, Vladimír - KAUPP, Martin. Scalar relativistic calculations of hyperfine coupling tensors using the Douglas-Kroll-Hess method with a finite-size nucleus model. In *Physical Chemistry Chemical Physics*, 2006, vol. 8, no. 35, p. 4079-4085. ISSN 1463-9076.

Citácie:

1. [1.1] AGUSTIN AUCAR, I. - GIMENEZ, Carlos A. - AUCAR, Gustavo A. Influence of the nuclear charge distribution and electron correlation effects on magnetic shieldings and spin-rotation tensors of linear molecules. In *RSC ADVANCES*. ISSN 2046-2069, 2018, vol. 8, no. 36, pp. 20234-20249., Registrované v: WOS
2. [1.1] SAITOW, Masaaki - NEESE, Frank. Accurate spin-densities based on the domain-based local pair-natural orbital coupled-cluster theory. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 3, pp., Registrované v: WOS

ADCA263 MALKIN, Irina - MALKINA, Oľga - MALKIN, Vladimír - KAUPP, Martin. Relativistic two-component calculations of electronic g-tensors that include spin polarization. In *Journal of Chemical Physics*, 2005, vol. 123, no. 24, p. 244103-1-244103-16. (2004: 3.105 - IF, karentované - CCC). (2005 - Current Contents, WOS, SCOPUS). ISSN 0021-9606.

Citácie:

1. [1.1] HAASE, Pi A. B. - REPISKY, Michal - KOMOROVSKY, Stanislav - BENDIX, Jesper - SAUER, Stephan P. A. Relativistic DFT Calculations of Hyperfine Coupling Constants in 5d Hexafluorido Complexes: [ReF₆](2-) and [IrF₆](2-). In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 20, pp. 5124-+, Registrované v: WOS
2. [1.1] SAYFUTYAROVA, Elvira R. - CHAN, Garnet Kin-Lic. Electron paramagnetic resonance g-tensors from state interaction spin-orbit coupling density matrix renormalization group. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 18, pp., Registrované v: WOS

ADCA264 MALKIN, Irina - MALKINA, Oľga - MALKIN, Vladimír - KAUPP, Martin. Scalar relativistic calculations of hyperfine coupling tensors using the Douglas-Kroll-Hess method. In *Chemical Physics Letters*, 2004, vol. 396, no. 4-6, p. 268-276.

Citácie:

1. [1.1] HAYAMI, Masao - SEINO, Junji - NAKAI, Hiromi. Gauge-origin independent formalism of two-component relativistic framework based on unitary transformation in nuclear magnetic shielding constant. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 11, pp., Registrované v: WOS

ADCA265 MALKIN, Vladimír - MALKINA, Oľga - ZHIDOMIROV, Georgy M. Visualization of electron paramagnetic resonance hyperfine structure coupling pathways. In *Journal of Physical Chemistry A. Molecules, spectroscopy, kinetics, environment, and general theory*, 2017, vol. 121, no. 18, p. 3580-3587. (2016: 2.847 - IF, Q2 - JCR, 1.252 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 1089-5639.

Citácie:

1. [1.1] WITWICKI, Maciej. Density functional theory and ab initio studies on hyperfine coupling constants of phosphinyl radicals. In *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY*. ISSN 0020-7608, 2018, vol. 118, no. 23, pp., Registrované v: WOS

- ADCA266 MALKIN, Vladimír - MALKINA, Oľga - SALAHUB, Dennis R. Spin-orbit correction to NMR shielding constants from density functional theory. In *Chemical Physics Letters*, 1996, vol. 261, no. 3, p. 335-345.
Citácie:
- [1.1] CHENG, Lan - WANG, Fan - STANTON, John F. - GAUSS, Juergen. Perturbative treatment of spin-orbit-coupling within spin-free exact two-component theory using equation-of-motion coupled-cluster methods. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 4, pp., Registrované v: WOS
 - [1.1] RUSAKOV, Yu. Yu. - RUSAKOVA, I. L. Relativistic heavy atom effect on C-13 NMR chemical shifts initiated by adjacent multiple chalcogens. In *MAGNETIC RESONANCE IN CHEMISTRY*. ISSN 0749-1581, 2018, vol. 56, no. 8, pp. 716-726., Registrované v: WOS
 - [1.1] RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic effects in the NMR spectra of compounds containing heavy chalcogens. In *MENDELEEV COMMUNICATIONS*. ISSN 0959-9436, 2018, vol. 28, no. 1, pp. 1-13., Registrované v: WOS
- ADCA267 MATEJDES, Marián - CZÍMEROVÁ, Adriana - JANEK, Marián. Fluorescence tuning of 2D montmorillonite optically active layers with beta-cyclodextrine/dye supramolecular complexes. In *Applied Clay Science*, 2015, vol. 114, p. 9-19. (2014: 2.467 - IF, Q1 - JCR, 0.918 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0169-1317.
Citácie:
- [1.1] BUJDAK, Juraj. Hybrids with Functional Dyes. In *INORGANIC NANOSHEETS AND NANOSHEET-BASED MATERIALS: FUNDAMENTALS AND APPLICATIONS OF TWO-DIMENSIONAL SYSTEMS*, 2017, vol., no., pp. 419-465., Registrované v: WOS
 - [1.1] WENG, Jianle - LIAO, Libing - LV, Guocheng - LI, Zhaohui - LI, Erwei - HE, Chun - WANG, Shuonan. Probing the interactions between lucigenin and phyllosilicates with different layer structures. In *DYES AND PIGMENTS*. ISSN 0143-7208, 2018, vol. 155, no., pp. 135-142., Registrované v: WOS
- ADCA268 MATUSIK, Jakub - SCHOLTZOVÁ, Eva - TUNEGA, Daniel. Influence of synthesis conditions on the formation of a kaolinite-methanol complex and simulation of its vibrational spectra. In *Clays and Clay Minerals*, 2012, vol. 60, no. 3, p. 227-239. (2011: 1.162 - IF, 0.696 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 0009-8604.
Citácie:
- [1.1] TABOROSI, Attila - SZILAGYI, Robert K. - ZSIRKA, Balazs - FONAGY, Orsolya - HORVATH, Erzsebet - KRISTOF, Janos. Molecular Treatment of Nano-Kaolinite Generations. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 12, pp. 7151-7167., Registrované v: WOS
 - [1.1] WANG, Ding - LIU, Qinfu - HOU, Dandan - ZHANG, Shuai - GUO, Peng - CHENG, Hongfei. Improved Method for Preparation of Methoxy-Modified Kaolinite. In *JOURNAL OF THE BRAZILIAN CHEMICAL SOCIETY*. ISSN 0103-5053, 2018, vol. 29, no. 1, pp. 33-37., Registrované v: WOS
- ADCA269 MIČOV, M. - TURI NAGY, L. - TUNEGA, Daniel - LIŠKA, Marek - PERICHTA, P. The structure and energetics of cryolite melts. In *Theoretical Chemistry Accounts*, 1998, vol. 99, no. 6, p. 378-383. ISSN 1432-881X.
Citácie:
- [1.1] BUCKO, Tomas - SIMKO, Frantisek. Effect of alkaline metal cations on the ionic structure of cryolite melts: Ab-initio NpT MD study. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 6, pp., Registrované v: WOS
- ADCA270 MICHÁLEK, Martin - SEDLÁČEK, Jaroslav - PARCHOVIANSKÝ, Milan - MICHÁLKOVÁ, Monika - GALUSEK, Dušan. Mechanical properties and electrical conductivity of alumina/MWCNT and alumina/zirconia/MWCNT composites. In *Ceramics International*, 2014, vol. 40, no. 1, p. 1289-1295. (2013: 2.086 - IF, 0.812 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 0272-8842.
Citácie:
- [1.1] HALDER, Rupa - SARKAR, Soumya - BANDYOPADHYAY, Siddhartha - CHAKRABORTI, Pravash C. Sintering and tribomechanical properties of gel-combustion-derived nano-alumina and its composites with carbon nanotubes. In *JOURNAL OF MATERIALS SCIENCE*. ISSN 0022-2461, 2018, vol. 53, no. 12, pp. 8989-9001., Registrované v: WOS
 - [1.1] IKRAM, Mujtaba - QAYYUM, H. A. - ALI, Sarmad - TAN, Ziqi - AHMAD, Muhammad - JIN, Xu. Hydrothermal-hot press processed SiO₂-rGO hybrid with enhanced physical properties. In *JOURNAL OF SOLID STATE CHEMISTRY*. ISSN 0022-4596, 2018, vol. 265, no., pp. 364-371., Registrované v: WOS
 - [1.1] IKRAM, Mujtaba - TAO, Zhuchen - YE, Jianglin - QAYYUM, Hafiz Adil - SUN, Xuemei - XU, Jin. Enhanced physical properties of gamma-Al₂O₃-rGO hybrids prepared by solvothermal and hot-press processing. In *RSC ADVANCES*. ISSN 2046-2069, 2018, vol. 8, no. 15, pp. 8329-8337., Registrované v: WOS
 - [1.1] ISLAM, Aminul - MUKHERJEE, Biswajyoti - SRIBALAJI, M. - RAHMAN, O. S. Asiq - ARUNKUMAR, P. - BABU, K. Suresh - KESHRI, Anup Kumar. Role of hybrid reinforcement of carbon nanotubes and graphene nanoplatelets on the electrical conductivity of plasma sprayed alumina coating. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 4, pp. 4508-4511., Registrované v: WOS
 - [1.1] KAYA, S. - AKCAN, D. - OZTURK, O. - ARDA, L. Enhanced mechanical properties of yttrium doped ZnO nanoparticles as determined by instrumented indentation technique. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 9, pp. 10306-10314., Registrované v: WOS
 - [1.1] LIN, Yan - WU, Shaohua - LI, Xiang - WU, Xin - YANG, Chunping - ZENG, Guangming - PENG, Yanrong - ZHOU, Qi - LU, Li. Microstructure and performance of Z-scheme photocatalyst of silver phosphate modified by MWCNTs and Cr-doped SrTiO₃ for malachite green degradation. In *APPLIED CATALYSIS B-ENVIRONMENTAL*. ISSN 0926-3373, 2018, vol. 227, no., pp. 557-570., Registrované v: WOS
 - [1.1] RAHMAN, O. S. Asiq - SRIBALAJI, M. - MUKHERJEE, Biswajyoti - LAHA, Tapas - KESHRI, Anup Kumar. Synergistic effect of hybrid carbon nanotube and graphene nanoplatelets reinforcement on processing, microstructure, interfacial stress and

mechanical properties of Al₂O₃ nanocomposites. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 2, pp. 2109-2122., Registrované v: WOS

8. [1.1] TOHIDIFAR, Mohammad Reza. Improving sintering behavior of MWCNT/BaTiO₃ ceramic nanocomposite with Bi₂O₃-B₂O₃ addition. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 4, pp. 3699-3706., Registrované v: WOS

ADCA271 MICHÁLEK, Martin - BODIŠOVÁ, Katarína - MICHÁLKOVÁ, Monika - SEDLÁČEK, Jaroslav - GALUSEK, Dušan. Alumina/MWCNTs composites by aqueous slip casting and pressureless sintering. In Ceramics International, 2013, vol. 39, no. 6, p. 6543-6550. (2012: 1.789 - IF, 0.816 - SJR, karentované - CCC). (2013 - Current Contents, WOS, SCOPUS). ISSN 0272-8842.(LPP-0297-09 : Keramické kompozity s perkolujúcimi fázami pripravené infiltráciou organokovového prekursoru. ITMS 26220120056 : Centrum excelentnosti pre keramiku, sklo a silikátové materiály).

Citácie:

1. [1.1] SCOTTI, Kristen L. - DUNAND, David C. Freeze casting A review of processing, microstructure and properties via the open data repository, FreezeCasting.net. In PROGRESS IN MATERIALS SCIENCE. ISSN 0079-6425, 2018, vol. 94, no., pp. 243-305., Registrované v: WOS

ADCA272 MICHÁLKOVÁ, Monika - GHILLÁNYOVÁ, Katarína - GALUSEK, Dušan. The influence of solid loading in suspensions of a submicrometric alumina powder on green and sintered pressure filtrated samples. In Ceramics International, 2010, vol. 36, no. 1, p. 385-390. (2009: 1.686 - IF, karentované - CCC). (2010 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] KUNCHALA, Pragnya - KAPPAGANTULA, Keerti. 3D printing high density ceramics using binder jetting with nanoparticle densifiers. In MATERIALS & DESIGN. ISSN 0264-1275, 2018, vol. 155, no., pp. 443-450., Registrované v: WOS

ADCA273 MICHÁLKOVÁ, Monika - KAŠIAROVÁ, Monika - TATARKO, Peter - DUSZA, Ján - ŠAJGALÍK, Pavol. Effect of homogenization treatment on the fracture behaviour of silicon nitride/graphene nanoplatelets composites. In Journal of the European Ceramic Society, 2014, vol. 34, no. 14, p. 3291-3299. (2013: 2.307 - IF, 1.122 - SJR, karentované - CCC). (2014 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] BASKUT, Sinem - CINAR, Alper - SEYHAN, A. Tugrul - TURAN, Servet. Tailoring the properties of spark plasma sintered SiAlON containing graphene nanoplatelets by using different exfoliation and size reduction techniques: Anisotropic electrical properties. In JOURNAL OF THE EUROPEAN CERAMIC SOCIETY. ISSN 0955-2219, 2018, vol. 38, no. 11, pp. 3787-3792., Registrované v: WOS

2. [1.1] CINAR, Alper - BASKUT, Sinem - SEYHAN, A. Tugrul - TURAN, Servet. Tailoring the properties of spark plasma sintered SiAlON containing graphene nanoplatelets by using different exfoliation and size reduction techniques: Anisotropic mechanical and thermal properties. In JOURNAL OF THE EUROPEAN CERAMIC SOCIETY. ISSN 0955-2219, 2018, vol. 38, no. 4, pp. 1299-1310., Registrované v: WOS

3. [1.1] LOPEZ-PERNIA, C. - MUNOZ-FERREIRO, C. - GONZALEZ-ORELLANA, C. - MORALES-RODRIGUEZ, A. - GALLARDO-LOPEZ, A. - POYATO, R. Optimizing the homogenization technique for graphene nanoplatelet/yttria tetragonal zirconia composites: Influence on the microstructure and the electrical conductivity. In JOURNAL OF ALLOYS AND COMPOUNDS. ISSN 0925-8388, 2018, vol. 767, no., pp. 994-1002., Registrované v: WOS

4. [1.1] WANG, Dongdong - SHAN, Zhongqiang - LIU, Xiaoyan - NA, Ren - WANG, Juan - LIU, Huitian - TIAN, Jianhua. High-rate Li₄Ti₅O₁₂/porous activated graphene nanoplatelets composites using LiOH both as lithium source and activating agent. In ELECTROCHIMICA ACTA. ISSN 0013-4686, 2018, vol. 262, no., pp. 9-17., Registrované v: WOS

5. [1.2] PORWAL, Harshit - SAGGAR, Richa. Ceramic matrix nanocomposites. In Comprehensive Composite Materials II, 2018-01-01, 6-8, pp. 138-161., Registrované v: SCOPUS

ADCA274 MIKULA, Marian - SANGIOVANNI, D. G. - PLAŠIENKA, D. - ROCH, T. - ČAPLOVIČOVÁ, M. - TRUHLÝ, M. - SATRAPINSKY, L. - BYSTRICKÝ, Roman - TONHAUZEROVÁ, D. - VLČKOVÁ, D. - KÚŠ, P. Thermally induced age hardening in tough Ta-Al-N coatings via spinodal decomposition. In Journal of Applied Physics, 2017, vol. 121, iss. 15, s. 155304-1 - 155304-7. (2016: 2.068 - IF, Q2 - JCR, 0.906 - SJR, Q2 - SJR, karentované - CCC). (2017 - Current Contents, WOS, SCOPUS). ISSN 0021-8979. Dostupné na internete: <<http://aip.scitation.org/doi/pdf/10.1063/1.4981534>>(APVV-14-0173 : Multikomponentné nanokompozitné povlaky pripravené vysokoionizovanými depozičnými technológiami).

Citácie:

1. [1.1] HAO, Jun - ZHANG, Yidan - REN, Ping - ZHANG, Kan - CHEN, Jianhong - DU, Suxuan - WANG, Meijia - WEN, Mao. Spinodal decomposition in the Ta-Mo-Al-N films activated by Mo incorporation: Toward enhanced hardness and toughness. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 17, pp. 21358-21364., Registrované v: WOS

2. [1.1] KINDLUND, Hanna - LU, Jun - BROITMAN, Esteban - PETROV, Ivan - GREENE, J. E. - BIRCH, Jens - HULTMAN, Lars. Growth and mechanical properties of 111-oriented V_{0.5}Mo_{0.5}Nx/Al₂O₃(0001) thin films. In JOURNAL OF VACUUM SCIENCE & TECHNOLOGY A. ISSN 0734-2101, 2018, vol. 36, no. 5, pp., Registrované v: WOS

3. [1.1] KOLLER, C. M. - MARIHART, H. - BOLVARDI, H. - KOLOZSVARI, S. - MAYRHOFER, P. H. Structure, phase evolution, and mechanical properties of DC, pulsed DC, and high power impulse magnetron sputtered Ta-N films. In SURFACE &

COATINGS TECHNOLOGY. ISSN 0257-8972, 2018, vol. 347, no., pp. 304-312., Registrované v: WOS

4. [1.1] POGREBNJAK, Alexander D. - IVASHCHENKO, Volodymyr I. - SKRYNSKYI, Petro L. - BONDAR, Oleksandr V. - KONARSKI, Piotr - ZALESKI, Karol - JURGA, Stefan - COY, Emerson. Experimental and theoretical studies of the physicochemical and mechanical properties of multi-layered TiN/SiC films: Temperature effects on the nanocomposite structure. In COMPOSITES PART B-ENGINEERING. ISSN 1359-8368, 2018, vol. 142, no., pp. 85-94., Registrované v: WOS

ADCA275 MILKO, Matúš - NOGA, Jozef - VARGA, Štefan. Accuracy of density fitting in calculation of two-electron repulsion integrals in periodic systems. In International Journal of Quantum Chemistry, 2007, vol. 107, no. 11, p. 2158-2168. (2006: 1.182 - IF). ISSN 0020-7608.

Citácie:

1. [1.1] SONG, Haigang - VAN DER VELDEN, Niels S. - SHIRAN, Sally L. - BLEIZIFFER, Patrick - ZACH, Christina - SIEBER, Ramon - IMANI, Aman S. - KRAUSBECK, Florian - AEBI, Markus - FREEMAN, Michael F. - RINIKER, Sereina - KUNZLER, Markus - NAISMITH, James H. A molecular mechanism for the enzymatic methylation of nitrogen atoms within peptide bonds. In SCIENCE ADVANCES. ISSN 2375-2548, 2018, vol. 4, no. 8, pp., Registrované v: WOS

ADCA276 MIŠKOVÁ, L. - LIŠKA, Marek - GALUSKOVÁ, Dagmar. Corrosion of E-glass fibers in distilled water. In Ceramics-Silikáty, 2007, vol. 51, no. 3, p. 131-135. (2006: 0.597 - IF, karentované - CCC). (2007 - Current Contents). ISSN 0862-5468.

Citácie:

1. [1.1] KRAUKLIS, Andrey E. - ECHTERMEYER, Andreas T. Long-Term Dissolution of Glass Fibers in Water Described by Dissolving Cylinder Zero-Order Kinetic Model: Mass Loss and Radius Reduction. In OPEN CHEMISTRY. ISSN 2391-5420, 2018, vol. 16, no. 1, pp. 1189-1199., Registrované v: WOS

ADCA277 MOJUMDAR, Subhash Chandra - RAY, A. - DRÁBIK, Milan - CIGÁŇ, Alexander - HANIC, František - CAPEK, Peter. Macro-Defect-Free (MDF) cements with high moisture resistance: chemical, thermal, SEM and magnetometric study. In Solid State Phenomena, 2003, vol. 90-91, p. 365-370. (2003 - Current Contents). ISSN 1012-0394.

Citácie:

1. [1.1] TOMAR, Priyanka - LAKHANI, Rajni - CHHIBBER, V. K. - KUMAR, Rajesh. Macro-defect free cements: a future oriented polymer composite materials for construction industries. In COMPOSITE INTERFACES. ISSN 0927-6440, 2018, vol. 25, no. 5-7, pp. 607-627., Registrované v: WOS

ADCA278 MÜLLER, Hendrik - KUTZELNIGG, Werner - NOGA, Jozef - KLOPPER, Wim. CH+5: The story goes on. An explicitly correlated coupled cluster study. In Journal of Chemical Physics, 1997, vol. 106, no. 5, p. 1863-1869. (1996: 3.516 - IF, karentované - CCC). (1997 - Current Contents, WOS, SCOPUS, WOS, SCOPUS). ISSN 0021-9606.

Citácie:

1. [1.1] ESSER, Alexander - FORBERT, Harald - MARX, Dominik. Tagging effects on the mid-infrared spectrum of microsolvated protonated methane. In CHEMICAL SCIENCE. ISSN 2041-6520, 2018, vol. 9, no. 6, pp. 1560-1573., Registrované v: WOS

2. [1.1] KWAN, Timothy - JORDAN, Meredith. The proton affinity of methane and its isotopologues: A test for theory. In CHEMICAL PHYSICS LETTERS. ISSN 0009-2614, 2018, vol. 708, no., pp. 216-221., Registrované v: WOS

3. [1.1] MONAJJEMI, M. Symmetry comparison of BH₅⁺ & CH₅⁺ ion and deuterated variants of BH₅D(5-x): real or artefactual stabilities. In MOROCCAN JOURNAL OF CHEMISTRY. ISSN 2351-812X, 2018, vol. 6, no. 4, pp. 588-600., Registrované v: WOS

4. [1.1] MONAJJEMI, Majid. Study of CD₅⁺ Ions and Deuterated Variants (CH₅D(5-x)⁺): An Artefactual Rotation. In RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 0036-0244, 2018, vol. 92, no. 11, pp. 2215-2226., Registrované v: WOS

ADCA279 NOGA, Jozef - KEDŽUCH, Stanislav - ŠIMUNEK, Ján - TEN-NO, Seiichiro. Explicitly correlated coupled cluster F12 theory with single and double excitations. In Journal of Chemical Physics, 2008, vol. 128, no. 17, p. 174103-1-174103-10. (2007: 3.044 - IF, karentované - CCC). (2008 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] GYORFFY, Werner - WERNER, Hans-Joachim. Analytical energy gradients for explicitly correlated wave functions. II. Explicitly correlated coupled cluster singles and doubles with perturbative triples corrections: CCSD(T)-F12. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 11, pp., Registrované v: WOS

2. [1.1] MA, Qianli - WERNER, Hans-Joachim. Explicitly correlated local coupled-cluster methods using pair natural orbitals. In WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE. ISSN 1759-0876, 2018, vol. 8, no. 6, pp., Registrované v: WOS

3. [1.1] MA, Qianli - WERNER, Hans-Joachim. Scalable Electron Correlation Methods. 5. Parallel Perturbative Triples Correction for Explicitly Correlated Local Coupled Cluster with Pair Natural Orbitals. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 1, pp. 198-215., Registrované v: WOS

4. [1.1] NAKATSUJI, Hiroshi - NAKASHIMA, Hiroyuki - KUOKAWA, Yusaku I. Solving the Schrodinger equation of atoms and molecules with the free-complement chemical-formula theory: First-row atoms and small molecules. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 11, pp., Registrované v: WOS

ADCA280 NOGA, Jozef - KEDŽUCH, Stanislav - ŠIMUNEK, Ján. Second order explicitly correlated R12 theory revisited: A second quantization framework for treatment of the operators'; partitionings. In Journal of Chemical Physics, 2007, vol. 127, no. 3, p. 034106-1-034106-11. (2007 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] GYORFFY, Werner - WERNER, Hans-Joachim. Analytical energy gradients for explicitly correlated wave functions. II. Explicitly correlated coupled cluster singles and doubles with perturbative triples corrections: CCSD(T)-F12. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 11, pp., Registrované v: WOS

2. [1.1] HEGELY, Bence - NAGY, Peter R. - KALLAY, Mihaly. Dual Basis Set Approach for Density Functional and Wave Function

Embedding Schemes. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 9, pp. 4600-4615., Registrované v: WOS

3. [1.1] MA, Qianli - WERNER, Hans-Joachim. Explicitly correlated local coupled-cluster methods using pair natural orbitals. In WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE. ISSN 1759-0876, 2018, vol. 8, no. 6, pp., Registrované v: WOS

4. [1.1] MA, Qianli - WERNER, Hans-Joachim. Scalable Electron Correlation Methods. 5. Parallel Perturbative Triples Correction for Explicitly Correlated Local Coupled Cluster with Pair Natural Orbitals. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 1, pp. 198-215., Registrované v: WOS

ADCA281 NOGA, Jozef - KUTZELNIGG, Werner - KLOPPER, Wim. CC-R12, a correlation cusp corrected coupled-cluster method with a pilot application to the Be2 potential curve. In Chemical Physics Letters, 1992, vol. 199, no. 5, p. 497-504.

Citácie:

1. [1.1] GYORFFY, Werner - WERNER, Hans-Joachim. Analytical energy gradients for explicitly correlated wave functions. II. Explicitly correlated coupled cluster singles and doubles with perturbative triples corrections: CCSD(T)-F12. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 11, pp., Registrované v: WOS

2. [1.1] KOPUT, Jacek. Ab initio potential energy surface and vibration-rotation energy levels of germanium dicarbide, GeC2. In JOURNAL OF COMPUTATIONAL CHEMISTRY. ISSN 0192-8651, 2018, vol. 39, no. 19, pp. 1327-1334., Registrované v: WOS

3. [1.1] MA, Qianli - WERNER, Hans-Joachim. Explicitly correlated local coupled-cluster methods using pair natural orbitals. In WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE. ISSN 1759-0876, 2018, vol. 8, no. 6, pp., Registrované v: WOS

4. [1.1] NAKATSUJI, Hiroshi - NAKASHIMA, Hiroyuki - KUOKAWA, Yusaku I. Solving the Schrodinger equation of atoms and molecules: Chemical-formula theory, free-complement chemical-formula theory, and intermediate variational theory. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 11, pp., Registrované v: WOS

5. [1.1] PRZYBYTEK, Michal - LESIUK, Michal. Correlation energies for many-electron atoms with explicitly correlated Slater functions. In PHYSICAL REVIEW A. ISSN 2469-9926, 2018, vol. 98, no. 6, pp., Registrované v: WOS

6. [1.1] PRZYBYTEK, Michal. Dispersion Energy of Symmetry-Adapted Perturbation Theory from the Explicitly Correlated F12 Approach. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 10, pp. 5105-5117., Registrované v: WOS

ADCA282 NOGA, Jozef - KUTZELNIGG, Werner. Coupled cluster theory that takes care of the correlation cusp by inclusion of linear terms in the interelectronic coordinates. In Journal of Chemical Physics, 1994, vol. 101, no. 9, p. 7738-7762. (1993: 3.615 - IF, karentované - CCC). (1994 - Current Contents, WOS, SCOPUS). ISSN 0021-9606.

Citácie:

1. [1.1] BARCA, Giuseppe M. J. - LOOS, Pierre-Francois. Recurrence Relations for Four-Electron Integrals Over Gaussian Basis Functions. In NOVEL ELECTRONIC STRUCTURE THEORY: GENERAL INNOVATIONS AND STRONGLY CORRELATED SYSTEMS. ISSN 0065-3276, 2018, vol. 76, no., pp. 147-165., Registrované v: WOS

2. [1.1] BOKHAN, Denis - TRUBNIKOV, Dmitrii N. - PERERA, Ajith - BARTLETT, Rodney J. Explicitly-correlated double ionization potentials and double electron attachment equation-of-motion coupled cluster methods. In CHEMICAL PHYSICS LETTERS. ISSN 0009-2614, 2018, vol. 692, no., pp. 191-195., Registrované v: WOS

3. [1.1] BOKHAN, Denis - TRUBNIKOV, Dmitrii N. - PERERA, Ajith - BARTLETT, Rodney J. Spin-orbit splitted excited states using explicitly-correlated equation-of-motion coupled-cluster singles and doubles eigenvectors. In CHEMICAL PHYSICS LETTERS. ISSN 0009-2614, 2018, vol. 698, no., pp. 171-175., Registrované v: WOS

4. [1.1] GYORFFY, Werner - WERNER, Hans-Joachim. Analytical energy gradients for explicitly correlated wave functions. II. Explicitly correlated coupled cluster singles and doubles with perturbative triples corrections: CCSD(T)-F12. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 11, pp., Registrované v: WOS

5. [1.1] KESHARWANI, Manoj K. - SYLVETSKY, Nitai - KOEHN, Andreas - TEW, David P. - MARTIN, Jan M. L. Do CCSD and approximate CCSD-F12 variants converge to the same basis set limits? The case of atomization energies. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 15, pp., Registrované v: WOS

6. [1.1] KOPUT, Jacek. Ab initio potential energy surface and vibration-rotation energy levels of germanium dicarbide, GeC2. In JOURNAL OF COMPUTATIONAL CHEMISTRY. ISSN 0192-8651, 2018, vol. 39, no. 19, pp. 1327-1334., Registrované v: WOS

7. [1.1] MA, Qianli - WERNER, Hans-Joachim. Explicitly correlated local coupled-cluster methods using pair natural orbitals. In WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE. ISSN 1759-0876, 2018, vol. 8, no. 6, pp., Registrované v: WOS

8. [1.1] TEW, David P. - KATS, Daniel. Relaxing Constrained Amplitudes: Improved F12 Treatments of Orbital Optimization and Core-Valence Correlation Energies. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 11, pp. 5435-5440., Registrované v: WOS

ADCA283 NOGA, Jozef - URBAN, Miroslav. On expectation value calculations of one-electron properties using the coupled cluster wave functions. In Theoretica Chimica Acta, 1988, vol. 73, no. 4, p. 291-306. ISSN 1432-881X.

Citácie:

1. [1.1] KOZLOWSKA, Justyna - SCHWILK, Max - ROZTOCZYNSKA, Agnieszka - BARTKOWIAK, Wojciech. Assessment of DFT for endohedral complexes; dipole moment: PNO-LCCSD-F12 as a reference method. In PHYSICAL CHEMISTRY CHEMICAL PHYSICS. ISSN 1463-9076, 2018, vol. 20, no. 46, pp. 29374-29388., Registrované v: WOS

2. [1.1] SAMANTA, Pradipta Kumar - KOEHN, Andreas. First-order properties from internally contracted multireference coupled-cluster theory with particular focus on hyperfine coupling tensors. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 6, pp., Registrované v: WOS

ADCA284 NOGA, Jozef - ŠIMUNEK, Ján. On the one-particle basis set relaxation in R12 based theories. In Chemical Physics, 2009, vol. 356, no. 1-3, p. 1-6. (2008: 1.961 - IF, karentované - CCC). (2009 -

Current Contents).

Citácie:

1. [1.1] KESHARWANI, Manoj K. - KARTON, Amir - SYLVETSKY, Nitai - MARTIN, Jan M. L. The S66 Non-Covalent Interactions Benchmark Reconsidered Using Explicitly Correlated Methods Near the Basis Set Limit. In AUSTRALIAN JOURNAL OF CHEMISTRY. ISSN 0004-9425, 2018, vol. 71, no. 4, pp. 238-248., Registrované v: WOS
2. [1.1] KESHARWANI, Manoj K. - MANNA, Debashree - SYLVETSKY, Nitai - MARTIN, Jan M. L. The X40x10 Halogen Bonding Benchmark Revisited: Surprising Importance of (n-1)d Subvalence Correlation. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 8, pp. 2184-2197., Registrované v: WOS
3. [1.1] PETERSON, Kirk A. - HILL, John Grant. On the Development of Accurate Gaussian Basis Sets for f-Block Elements. In ANNUAL REPORTS IN COMPUTATIONAL CHEMISTRY, VOL 14, ISSN 1574-1400, 2018, vol. 14, no., pp. 47-74., Registrované v: WOS

ADCA285

NOGA, Jozef - BARTLETT, Rodney J. - URBAN, Miroslav. Towards a full CCSDT model for electron correlation. CCSDT-n models. In Chemical Physics Letters, 1987, vol. 134, no. 2, p. 126-132.

Citácie:

1. [1.1] LISCHKA, Hans - NACHTIGALLOVA, Dana - AQUINO, Adelia J. A. - SZALAY, Peter G. - PLASSER, Felix - MACHADO, Francisco B. C. - BARBATTI, Mario. Multireference Approaches for Excited States of Molecules. In CHEMICAL REVIEWS. ISSN 0009-2665, 2018, vol. 118, no. 15, pp. 7293-7361., Registrované v: WOS

ADCA286

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

Citácie:

1. [1.1] ALESSANDRINI, Silvia - GAUSS, Juergen - PUZZARINI, Cristina. Accuracy of Rotational Parameters Predicted by High-Level Quantum-Chemical Calculations: Case Study of Sulfur-Containing Molecules of Astrochemical Interest. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 10, pp. 5360-5371., Registrované v: WOS
2. [1.1] BARTLETT, Marcus A. - LIANG, Tao - PU, Liang - SCHAEFER, Henry F. - ALLEN, Wesley D. The multichannel n-propyl + O-2 reaction surface: Definitive theory on a model hydrocarbon oxidation mechanism. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 9, pp., Registrované v: WOS
3. [1.1] BAUSCHLICHER, Charles W. The convergence of the coupled cluster approach for MgO. In CHEMICAL PHYSICS LETTERS. ISSN 0009-2614, 2018, vol. 711, no., pp. 27-31., Registrované v: WOS
4. [1.1] BICZYSKO, Malgorzata - BLOINO, Julien - PUZZARINI, Cristina. Computational challenges in Astrochemistry. In WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE. ISSN 1759-0876, 2018, vol. 8, no. 3, pp., Registrované v: WOS
5. [1.1] CROCE, Adela E. - COBOS, Carlos J. Quantum-chemical and kinetic study of the reactions of the ClSO₂ radical with H, O, Cl, S, SCl and ClSO₂ in the atmosphere of Venus. In COMPUTATIONAL AND THEORETICAL CHEMISTRY. ISSN 2210-271X, 2018, vol. 1140, no., pp. 14-23., Registrované v: WOS
6. [1.1] IVANIC, Joseph - SCHMIDT, Michael W. Hybrid Correlation Energy (HyCE): An Approach Based on Separate Evaluations of Internal and External Components. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 23, pp. 5223-5237., Registrované v: WOS
7. [1.1] KOWALSKI, Karol - BRABEC, Jiri - PENG, Bo. Regularized and Renormalized Many-Body Techniques for Describing Correlated Molecular Systems: A Coupled-Cluster Perspective. In ANNUAL REPORTS IN COMPUTATIONAL CHEMISTRY, VOL 14, ISSN 1574-1400, 2018, vol. 14, no., pp. 3-45., Registrované v: WOS
8. [1.1] KOWALSKI, Karol. Properties of coupled-cluster equations originating in excitation sub-algebras. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 9, pp., Registrované v: WOS
9. [1.1] KUMAR, Manoj - LI, Hao - ZHANG, Xiuhui - ZENG, Xiao Cheng - FRANCISCO, Joseph S. Nitric Acid-Amine Chemistry in the Gas Phase and at the Air-Water Interface. In JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. ISSN 0002-7863, 2018, vol. 140, no. 20, pp. 6456-6466., Registrované v: WOS
10. [1.1] KUMAR, Manoj - SAIZ-LOPEZ, Alfonso - FRANCISCO, Joseph S. Single-Molecule Catalysis Revealed: Elucidating the Mechanistic Framework for the Formation and Growth of Atmospheric Iodine Oxide Aerosols in Gas-Phase and Aqueous Surface Environments. In JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. ISSN 0002-7863, 2018, vol. 140, no. 44, pp. 14704-14716., Registrované v: WOS
11. [1.1] KUMAR, Ragesh T. P. - BRYNJARSSON, B. - OMARSSON, B. - HOSHINO, M. - TANAKA, H. - LIMA-VIEIRA, P. - JONES, D. B. - BRUNGER, M. J. - INGOLFSSON, O. Negative ion formation through dissociative electron attachment to the group IV tetrachlorides: Carbon tetrachloride, silicon tetrachloride and germanium tetrachloride. In INTERNATIONAL JOURNAL OF MASS SPECTROMETRY. ISSN 1387-3806, 2018, vol. 426, no., pp. 12-28., Registrované v: WOS
12. [1.1] LISCHKA, Hans - NACHTIGALLOVA, Dana - AQUINO, Adelia J. A. - SZALAY, Peter G. - PLASSER, Felix - MACHADO, Francisco B. C. - BARBATTI, Mario. Multireference Approaches for Excited States of Molecules. In CHEMICAL REVIEWS. ISSN 0009-2665, 2018, vol. 118, no. 15, pp. 7293-7361., Registrované v: WOS
13. [1.1] LOOS, Pierre-Francois - SCEMAMA, Anthony - BLONDEL, Aymeric - GARNIRON, Yann - CAFFAREL, Michel - JACQUEMIN, Denis. A Mountaineering Strategy to Excited States: Highly Accurate Reference Energies and Benchmarks. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 8, pp. 4360-4379., Registrované v: WOS
14. [1.1] MAGOULAS, Ilias - BAUMAN, Nicholas P. - SHEN, Jun - PIECUCH, Piotr. Application of the CC(P;Q) Hierarchy of Coupled Cluster Methods to the Beryllium Dimer. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 5, pp. 1350-1368., Registrované v: WOS
15. [1.1] MORGAN, W. James - MATTHEWS, Devin A. - RINGHOLM, Magnus - AGARWAL, Jay - GONG, Justin Z. - RUUD, Kenneth - ALLEN, Wesley D. - STANTON, John F. - SCHAEFER, Henry F. Geometric Energy Derivatives at the Complete Basis Set Limit: Application to the Equilibrium Structure and Molecular Force Field of Formaldehyde. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 3, pp. 1333-1350., Registrované v: WOS

16. [1.1] PARANDAMAN, Arathala - KUMAR, Manoj - FRANCISCO, Joseph S. - SINHA, Amitabha. Organic Acid Formation from the Atmospheric Oxidation of Gem Diols: Reaction Mechanism, Energetics, and Rates. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 30, pp. 6266-6276., Registrované v: WOS
 17. [1.1] PARANDAMAN, Arathala - PEREZ, Josue E. - SINHA, Amitabha. Atmospheric Decomposition of Trifluoromethanol Catalyzed by Formic Acid. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 49, pp. 9553-9562., Registrované v: WOS
 18. [1.1] ROLIK, Zoltan - KALLAY, Mihaly. Novel strategy to implement active-space coupled-cluster methods. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 148, no. 12, pp., Registrované v: WOS
 19. [1.1] RUSAKOV, Yury Yu - RUSAKOVA, Irina L. - SEMENOV, Valentin A. - SAMULTSEV, Dmitry O. - FEDOROV, Sergei V. - KRIVDIN, Leonid B. Calculation of N-15 and P-31 NMR Chemical Shifts of Azoles, Phospholes, and Phosphazoles: A Gateway to Higher Accuracy at Less Computational Cost. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 33, pp. 6746-6759., Registrované v: WOS
 20. [1.1] SCEMAMA, Anthony - BENALI, Anouar - JACQUEMIN, Denis - CAFFAREL, Michel - LOOS, Pierre-Francois. Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 3, pp., Registrované v: WOS
 21. [1.1] TASI, Domonkos A. - FABIAN, Zita - CZAKO, Gabor. Benchmark ab Initio Characterization of the Inversion and Retention Pathways of the OH- + CH3Y [Y = F, Cl, Br, I] S(N)2 Reactions. In JOURNAL OF PHYSICAL CHEMISTRY A. ISSN 1089-5639, 2018, vol. 122, no. 26, pp. 5773-5780., Registrované v: WOS
 22. [1.1] TRAN, Henry K. - STANTON, John F. - MILLER, Terry A. Quantifying the effects of higher order coupling terms on fits using a second order Jahn-Teller Hamiltonian. In JOURNAL OF MOLECULAR SPECTROSCOPY. ISSN 0022-2852, 2018, vol. 343, no., pp. 102-115., Registrované v: WOS
 23. [1.1] XU, Enhua - TEN-NO, Seiichiro L. Partially linearized external models to active-space coupled-cluster through connected hextuple excitations. In JOURNAL OF COMPUTATIONAL CHEMISTRY. ISSN 0192-8651, 2018, vol. 39, no. 15, pp. 875-880., Registrované v: WOS
 24. [1.1] ZHOU, Dan - LI, Guoliang - MOORE, Kevin B. - XIE, Yaoming - PETERSON, Kirk A. - SCHAEFER, Henry F. Noncovalent Interactions between Molecular Hydrogen and the Alkali Fluorides: H-H center dot center dot center dot F-M (M = Li, Na, K, Rb, Cs). High Level Theoretical Predictions and SAPT Analysis. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 10, pp. 5118-5127., Registrované v: WOS
- ADCA287 NOVOTNÝ, Jan - VÍCHA, Jan - BORA, Pankaj L. - REPISKÝ, Michal - STRAKA, Michal - KOMOROVSKÝ, Stanislav - MAREK, Radek. Linking the character of the metal-ligand bond to the ligand NMR shielding in transition-metal complexes: NMR contributions from spin-orbit coupling. In Journal of Chemical Theory and Computation, 2017, vol. 13, no. 8, p. 3586-3601. (2016: 5.245 - IF, Q1 - JCR, 2.711 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 1549-9618.

Citácie:

1. [1.1] GORDON, Christopher P. - SHIRASE, Satoru - YAMAMOTO, Keishi - ANDERSEN, Richard A. - EISENSTEIN, Odile - COPERET, Christophe. NMR chemical shift analysis decodes olefin oligo- and polymerization activity of d(0) group 4 metal complexes. In PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA. ISSN 0027-8424, 2018, vol. 115, no. 26, pp. E5867-E5876., Registrované v: WOS
 2. [1.1] GORDON, Christopher P. - YAMAMOTO, Keishi - SEARLES, Keith - SHIRASE, Satoru - ANDERSEN, Richard A. - EISENSTEIN, Odile - COPERET, Christophe. Metal alkyls programmed to generate metal alkylidenes by alpha-H abstraction: prognosis from NMR chemical shift. In CHEMICAL SCIENCE. ISSN 2041-6520, 2018, vol. 9, no. 7, pp. 1912-1918., Registrované v: WOS
 3. [1.1] LI, Xinying - CAO, Xue. On the covalence in H-2 AuX (X = F-I). In INTERNATIONAL JOURNAL OF HYDROGEN ENERGY. ISSN 0360-3199, 2018, vol. 43, no. 3, pp. 1709-1717., Registrované v: WOS
 4. [1.1] ROCCHIGIANI, Luca - FERNANDEZ-CESTAU, Julio - CHAMBRIER, Isabelle - HROBARIK, Peter - BOCHMANN, Manfred. Unlocking Structural Diversity in Gold(III) Hydrides: Unexpected Interplay of cis/trans-Influence on Stability, Insertion Chemistry, and NMR Chemical Shifts. In JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. ISSN 0002-7863, 2018, vol. 140, no. 26, pp. 8287-8302., Registrované v: WOS
 5. [1.1] RUSAKOV, Yu. Yu. - RUSAKOVA, I. L. Relativistic heavy atom effect on C-13 NMR chemical shifts initiated by adjacent multiple chalcogens. In MAGNETIC RESONANCE IN CHEMISTRY. ISSN 0749-1581, 2018, vol. 56, no. 8, pp. 716-726., Registrované v: WOS
 6. [1.1] RUSAKOV, Yury Yu - RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic heavy atom effect on the P-31 NMR parameters of phosphine chalcogenides. Part 1. Chemical shifts. In MAGNETIC RESONANCE IN CHEMISTRY. ISSN 0749-1581, 2018, vol. 56, no. 11, pp. 1061-1073., Registrované v: WOS
 7. [1.1] RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic effects in the NMR spectra of compounds containing heavy chalcogens. In MENDELEEV COMMUNICATIONS. ISSN 0959-9436, 2018, vol. 28, no. 1, pp. 1-13., Registrované v: WOS
 8. [1.1] SHAKOORIOSKOOIE, Mandieh - MENCELOGLU, Yusuf Z. - UNAL, Serkan - SOYTAS, Serap Hayat. Rapid Microwave-Assisted Synthesis of Platinum Nanoparticles Immobilized in Electrospun Carbon Nanofibers for Electrochemical Catalysis. In ACS APPLIED NANO MATERIALS. ISSN 2574-0970, 2018, vol. 1, no. 11, pp. 6236-6246., Registrované v: WOS
- ADCA288 NOVOTNÝ, Jan - PŘICHYSTAL, David - SOJKA, Martin - KOMOROVSKÝ, Stanislav - NEČAS, Marek - MAREK, Radek. Hyperfine effects in ligand NMR: Paramagnetic Ru(III) complexes with 3-substituted pyridines. In Inorganic Chemistry, 2018, vol. 57, no. 2, p. 641-652. (2017: 4.700 - IF, Q1 - JCR, 1.892 - SJR, Q1 - SJR, karentované - CCC). (2018 - Current Contents, WOS, SCOPUS). ISSN 0020-1669.

Citácie:

1. [1.1] MARES, Jiri - VAARA, Juha. Ab initio paramagnetic NMR shifts via point- dipole approximation in a large magnetic- anisotropy Co(II) complex. In PHYSICAL CHEMISTRY CHEMICAL PHYSICS. ISSN 1463-9076, 2018, vol. 20, no. 35, pp. 22547-22555., Registrované v: WOS

2. [1.1] SERGENTU, Dumitru-Claudiu - GENDRON, Frederic - AUTSCHBACH, Jochen. Similar ligand-metal bonding for transition metals and actinides? 5f(1) U(C7H7)(2)(-) versus 3d(n) metallocenes. In *CHEMICAL SCIENCE*. ISSN 2041-6520, 2018, vol. 9, no. 29, pp. 6292-6306., Registrované v: WOS

ADCA289 OREŠKOVÁ, Gabriela - CHRAPPOVÁ, Jana - PUŠKELOVÁ, Jarmila - ŠIMUNEK, Ján - SCHWENDT, Peter - NOGA, Jozef - GYEPES, Róbert. Synthesis, crystal structure, spectral characterization, and theoretical study of glycolato peroxido complexes of vanadium(V). In *Structural Chemistry*, 2016, vol. 27, no. 2, p. 605-615. (2015: 1.854 - IF, Q2 - JCR, 0.539 - SJR, Q2 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 1040-0400.

Citácie:

1. [1.1] MCLAUCHLAN, Craig C. - MURAKAMI, Heide A. - WALLACE, Craig A. - CRANS, Debbie C. Coordination environment changes of the vanadium in vanadium-dependent haloperoxidase enzymes. In *JOURNAL OF INORGANIC BIOCHEMISTRY*. ISSN 0162-0134, 2018, vol. 186, no., pp. 267-279., Registrované v: WOS

ADCA290 OSACKÝ, Marek - ŠUCHA, Vladimír - CZÍMEROVÁ, Adriana - MADEJOVÁ, Jana. Reaction of smectites with iron in a nitrogen atmosphere at 75 °C. In *Applied Clay Science*, 2010, vol. 50, no. 2, p. 237-244. (2009: 2.784 - IF, karentované - CCC). (2010 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] CHESHIRE, M. C. - CAPORUSCIO, F. A. - COLON, C. F. Jove - NORSKOG, K. E. Fe-saponite growth on low-carbon and stainless steel in hydrothermal-bentonite experiments. In *JOURNAL OF NUCLEAR MATERIALS*. ISSN 0022-3115, 2018, vol. 511, no., pp. 353-366., Registrované v: WOS

ADCA291 OSACKÝ, Marek - ŠUCHA, Vladimír - CZÍMEROVÁ, Adriana - PENTRÁK, Martin - MADEJOVÁ, Jana. Reaction of smectites with iron in aerobic conditions at 75 °C. In *Applied Clay Science*, 2013, vol. 72, p. 26-36. (2012: 2.342 - IF, 1.118 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 0169-1317. (Vega č. 2/0183/09 : Chemické modifikácie povrchov prírodných nanomateriálov. Vega č. 2/0089/09 : Fluorescenčné hybridné materiály organických farbív interkalovaných v anorganických nosičoch s vrstevnatou štruktúrou. ITMS 26240120007 : Centrum pre materiály, vrstvy a systémy pre aplikácie a chemické procesy v extrémnych podmienkach).

Citácie:

1. [1.1] DZENE, Liva - BRENDLE, Jocelyne - LIMOUSY, Lionel - DUTOURNIE, Patrick - MARTIN, Christelle - MICHAU, Nicolas. Synthesis of iron-rich tri-octahedral clay minerals: A review. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 166, no., pp. 276-287., Registrované v: WOS

2. [1.1] POLAK, Filip - URIK, Martin - BUJDOS, Marek - UHLIK, Peter - MATUS, Peter. Evaluation of aluminium mobilization from its soil mineral pools by simultaneous effect of *Aspergillus* strains; acidic and chelating exometabolites. In *JOURNAL OF INORGANIC BIOCHEMISTRY*. ISSN 0162-0134, 2018, vol. 181, no., pp. 162-168., Registrované v: WOS

ADCA292 PÁLKOVÁ, Helena - MADEJOVÁ, Jana - ZIMOWSKA, Malgorzata - SERWICKA, Ewa M. Laponite-derived porous clay heterostructures: II. FTIR study of the structure evolution. In *Microporous and Mesoporous Materials*, 2010, vol. 127, no. 3, p. 237-244. (2009: 2.652 - IF).

Citácie:

1. [1.1] CECILIA, J. A. - GARCIA-SANCHO, C. - VILARRASA-GARCIA, E. - JIMENEZ-JIMENEZ, J. - RODRIGUEZ-CASTELLON, E. Synthesis, Characterization, Uses and Applications of Porous Clays Heterostructures: A Review. In *CHEMICAL RECORD*. ISSN 1527-8999, 2018, vol. 18, no. 7-8, pp. 1085-1104., Registrované v: WOS

2. [1.1] CHRISTIDIS, George E. - ALDANA, Carlos - CHRYSSIKOS, Georgios D. - GIONIS, Vassilis - KALO, Hussein - STOETER, Matthias - BREU, Josef - ROBERT, Jean-Louis. The Nature of Laponite: Pure Hectorite or a Mixture of Different Trioctahedral Phases? In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 8, pp., Registrované v: WOS

3. [1.1] LI JING - CUI JIN-CAN - YANG ZHEN-ZHEN - QIU HAN-XUN - TANG ZHI-HONG - YANG JUN-HE. Stabilizing graphene layers by intercalating laponite between them. In *NEW CARBON MATERIALS*. ISSN 1007-8827, 2018, vol. 33, no. 1, pp. 19-25., Registrované v: WOS

4. [1.1] SHI, Jiabo - WANG, Chunhua - NGAI, To - LIN, Wei. Diffusion and Binding of Laponite Clay Nanoparticles into Collagen Fibers for the Formation of Leather Matrix. In *LANGMUIR*. ISSN 0743-7463, 2018, vol. 34, no. 25, pp. 7379-7385., Registrované v: WOS

5. [1.1] TULLI, Fiorella - GULOTTA, Florencia A. - MARTINO, Debora M. - PAZ ZANINI, Veronica I. - BORSARELLI, Claudio D. Ultrasensitive Amperometric Biosensing of Polyphenols Using Horseradish Peroxidase Immobilized in a Laponite/Au/DNA-Bioinspired Polycation Nanocomposite. In *JOURNAL OF THE ELECTROCHEMICAL SOCIETY*. ISSN 0013-4651, 2018, vol. 165, no. 10, pp. B452-B457., Registrované v: WOS

ADCA293 PÁLKOVÁ, Helena - MADEJOVÁ, Jana - ZIMOWSKA, Malgorzata - BIELAŃSKA, Elzbieta - OLEJNICZAK, Zbigniew - LITYŃSKA-DOBRYŃSKA, Lidia - SERWICKA, Ewa M. Laponite-derived porous clay heterostructures: I. Synthesis and physicochemical characterization. In *Microporous and Mesoporous Materials*, 2010, vol. 127, no. 3, p. 228-236. (2009: 2.652 - IF).

Citácie:

1. [1.1] CECILIA, J. A. - GARCIA-SANCHO, C. - VILARRASA-GARCIA, E. - JIMENEZ-JIMENEZ, J. - RODRIGUEZ-CASTELLON, E. Synthesis, Characterization, Uses and Applications of Porous Clays Heterostructures: A Review. In *CHEMICAL RECORD*. ISSN 1527-8999, 2018, vol. 18, no. 7-8, pp. 1085-1104., Registrované v: WOS

ADCA294 PÁLKOVÁ, Helena - HRONSKÝ, Viktor - JANKOVIČ, Ľuboš - MADEJOVÁ, Jana. The effect of acid treatment on the structure and surface acidity of tetraalkylammonium-montmorillonites. In *Journal of Colloid and Interface Science*, 2013, vol. 395, p. 166-175. (2012: 3.172 - IF, 1.298 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 0021-9797. (APVV-0362-10 : Organofly a ich kompozity s polymérmi. Vega č. 2/0183/09 : Chemické modifikácie povrchov prírodných nanomateriálov).

Citácie:

1. [1.1] LIU, Zhengjiang - MA, Huiyan - LIU, Juming - XING, Lei - CHENG, Lin - YANG, Jucai - MAO, Baodong - ZHANG, Qiancheng. A low-cost clay-based heterogeneous Fenton-like catalyst: Activation, efficiency enhancement, and mechanism study. In *ASIA-PACIFIC JOURNAL OF CHEMICAL ENGINEERING*. ISSN 1932-2135, 2018, vol. 13, no. 1, pp., Registrované v: WOS

ADCA295 PÁLKOVÁ, Helena - HRONSKÝ, Viktor - BIZOVSKÁ, Valéria - MADEJOVÁ, Jana. Spectroscopic study of water adsorption on Li⁺, TMA⁺ and HDTMA⁺ exchanged montmorillonite. In *Spectrochimica Acta Part A - Molecular and Biomolecular Spectroscopy*, 2015, vol. 149, p. 751-761. (2014: 2.353 - IF, Q2 - JCR, 0.626 - SJR, Q2 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 1386-1425.

Citácie:

1. [1.1] NADERI, Arman - DELAVAR, Mohammad Amir - GHORBANI, Yousef - KABOUDIN, Babak - HOSSEINI, Mehdi. Modification of nano-clays with ionic liquids for the removal of Cd (II) ion from aqueous phase. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 158, no., pp. 236-245., Registrované v: WOS

2. [1.1] PAUL, Geo - BISIO, Chiara - BRASCHI, Ilaria - COSSI, Maurizio - GATTI, Giorgio - GIANOTTI, Enrica - MARCHESE, Leonardo. Combined solid-state NMR, FT-IR and computational studies on layered and porous materials. In *CHEMICAL SOCIETY REVIEWS*. ISSN 0306-0012, 2018, vol. 47, no. 15, pp. 5684-5739., Registrované v: WOS

ADCA296 PÁLKOVÁ, Helena - ZIMOWSKA, Malgorzata - JANKOVIČ, Ľuboš - SULIKOWSKI, B. - SERWICKA, Ewa M. - MADEJOVÁ, Jana. Thermal stability of tetrabutyl-phosphonium and - ammonium exchanged montmorillonite: Influence of acid treatment. In *Applied Clay Science*, 2017, vol. 138, p. 63-73. (2016: 3.101 - IF, Q1 - JCR, 0.899 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] BUJDAKOVA, H. - BUJDAKOVA, V. - MAJEKOVA-KOSCOVA, H. - GAALOVA, B. - BIZOVSKA, V. - BOHAC, P. - BUJDAK, J. Antimicrobial activity of organoclays based on quaternary alkylammonium and alkylphosphonium surfactants and montmorillonite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 158, no., pp. 21-28., Registrované v: WOS

2. [1.2] ABDULLAH, M. A.A. - MAMAT, M. - RUSLI, S. A. - KASSIM, A. A. Influence of Alkylphosphonium modified montmorillonite to the tensile properties of PMMA composites. In *ASM Science Journal*. ISSN 18236782, 2018-01-01, 11, special Issue 1, pp. 96-104., Registrované v: SCOPUS

ADCA297 PARCHOVIANSKÝ, Milan - GALUSEK, Dušan - MICHÁLEK, Martin - ŠVANČÁREK, Peter - KAŠIAROVÁ, Monika - DUSZA, Ján - HNATKO, Miroslav. Effect of the volume fraction of SiC on the microstructure and creep behavior of hot pressed Al₂O₃/SiC composites. In *Ceramics International*, 2014, vol. 40, no. 1, p. 1807-1814. (2013: 2.086 - IF, 0.812 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] CHO, Seulki - PARK, Sung-Joon - MIN, Seong-Ji - AN, Jae-In - YOON, Yo-Seop - MOON, Byungmoo - CHOI, Youngwoong - LEE, Sang-Kwon - KOO, Sang-Mo. SiC Nanopowders-Incorporated Dual-Channel TiZnSnO/ZnSnO Thin Film Transistors. In *NANOSCIENCE AND NANOTECHNOLOGY LETTERS*. ISSN 1941-4900, 2018, vol. 10, no. 11, pp. 1562-1566., Registrované v: WOS

2. [1.1] HENNICHE, Abdelkhalek - OUYANG, Jia Hu - LIU, Zhan Guo - MA, Yong Hui - WANG, Zhi Gang - WANG, Yu Jin - DERRADJI, Mehdi. Effect of SiC addition on mechanical properties of hot-pressed AlO-GdAlOO-ceramics with eutectic composition. In *Ceramics International*. ISSN 02728842, 2018-06-01, 44, 8, pp. 9585-9592., Registrované v: WOS

3. [1.1] LAO, Xinbin - XU, Xiaoyang. Effect of silica on in-situ synthesis of nano-SiC whiskers in porous Al₂O₃-SiC composite ceramics for solar thermal storage by aluminium-assisted carbothermal reduction. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 16, pp. 20501-20507., Registrované v: WOS

ADCA298 PARCHOVIANSKÝ, Milan - GALUSEK, Dušan - SEDLÁČEK, Jaroslav - ŠVANČÁREK, Peter - KAŠIAROVÁ, Monika - DUSZA, Ján - ŠAJGALÍK, Pavol. Microstructure and mechanical properties of hot pressed Al₂O₃/SiC nanocomposites. In *Journal of the European Ceramic Society*, 2013, vol. 33, no. 12, p. 2291-2298. (2012: 2.360 - IF, 1.305 - SJR, karentované - CCC). (2013 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.(LPP-0297-09 : Keramické kompozity s perkolujúcimi fázami pripravené infiltráciou organokovového prekursoru. ITMS 26220120056 : Centrum excelentnosti pre keramiku, sklo a silikátové materiály).

Citácie:

1. [1.1] AI, Yunlong - LIU, Ying - ZHANG, Qiuyu - GONG, Yuxing - HE, Wen - ZHANG, Jianjun. Microwave Sintering of Graphene-Nanoplatelet-Reinforced Al₂O₃-based Composites. In *JOURNAL OF THE KOREAN CERAMIC SOCIETY*. ISSN 1229-7801, 2018, vol. 55, no. 6, pp. 556-561., Registrované v: WOS

2. [1.1] ELYAS, Hawsawi - KIM, Tae Woo - JANG, Byung-Koog - LEE, Kee Sung. Damage and wear resistance of Al₂O₃-SiC microcomposites with hard and elastic properties. In *JOURNAL OF THE CERAMIC SOCIETY OF JAPAN*. ISSN 1882-0743, 2018, vol. 126, no. 1, pp. 21-26., Registrované v: WOS

3. [1.1] HENNICHE, Abdelkhalek - OUYANG, Jia Hu - LIU, Zhan Guo - MA, Yong Hui - WANG, Zhi Gang - WANG, Yu Jin - DERRADJI, Mehdi. Effect of SiC addition on mechanical properties of hot-pressed AlO-GdAlOO-ceramics with eutectic composition. In *Ceramics International*. ISSN 02728842, 2018-06-01, 44, 8, pp. 9585-9592., Registrované v: WOS

4. [1.1] KOU, Gang - GUO, Ling jun - LIU, Ning kun - CHEN, Miao miao - XU, Min - ZHAO, Zhi gang. Significant influence of AlO-on the flexural properties of C/C composites. In *Vacuum*. ISSN 0042207X, 2018-05-01, 151, pp. 294-297., Registrované v: WOS

5. [1.1] MICHALEK, Martin - MICHALKOVA, Monika - BLUGAN, Gurdial - KUEBLER, Jakob. Strength of pure alumina ceramics above 1 GPa. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 3, pp. 3255-3260., Registrované v:

WOS

6. [1.1] YE, C. L. - LIOU, G. T. Effects of PTFE activation and excess Al on combustion synthesis of SiC-and ZrC-Al₂O₃ composites. In VACUUM. ISSN 0042-207X, 2018, vol. 154, no., pp. 186-189., Registrované v: WOS

7. [1.1] ZHOU, Weiwei - SUN, Xiaohao - KIKUCHI, Keiko - NOMURA, Naoyuki - YOSHIMI, Kyosuke - KAWASAKI, Akira. Carbon nanotubes as a unique agent to fabricate nanoceramic/metal composite powders for additive manufacturing. In MATERIALS & DESIGN. ISSN 0264-1275, 2018, vol. 137, no., pp. 276-285., Registrované v: WOS

8. [1.2] KUMAR, Sandeep - SARITA - NEHRA, Monika - DILBAGHI, Neeraj - TANKESHWAR, K. - KIM, Ki Hyun. Recent advances and remaining challenges for polymeric nanocomposites in healthcare applications. In Progress in Polymer Science. ISSN 0079-6700, 2018-05-01, 80, pp. 1-38., Registrované v: SCOPUS

9. [1.2] MAITRA, Saikat - ROY, Jagannath. Nanoceramic matrix composites: Types, processing, and applications. In Advances in Ceramic Matrix Composites: Second Edition, 2018-01-20, pp. 27-48., Registrované v: SCOPUS

ADCA299 PARCHOVIANSKÝ, Milan - BALKO, Ján - ŠVANČÁREK, Peter - SEDLÁČEK, Jaroslav - DUSZA, Ján - LOFAJ, František - GALUSEK, Dušan. Mechanical properties and sliding wear behaviour of Al₂O₃-SiC nanocomposites with 3-20 vol% SiC. In Journal of the European Ceramic Society, 2017, vol. 37, p. 4297-4306. (2016: 3.454 - IF, Q1 - JCR, 1.142 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0955-2219.

Citácie:

1. [1.1] ELYAS, Hawsawi - KIM, Tae Woo - JANG, Byung-Koog - LEE, Kee Sung. Damage and wear resistance of Al₂O₃-SiC microcomposites with hard and elastic properties. In JOURNAL OF THE CERAMIC SOCIETY OF JAPAN. ISSN 1882-0743, 2018, vol. 126, no. 1, pp. 21-26., Registrované v: WOS

2. [1.1] LI, Zhenbao - CAO, Yejie - HE, Jiabei - WANG, Yiguang. Mechanical and tribological performances of C-SiC nanocomposites synthesized from polymer-derived ceramics sintered by spark plasma Check for sintering. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 12, pp. 14335-14341., Registrované v: WOS

3. [1.1] NATRAYAN, L. - KUMAR, M. Senthil - PALANIKUMAR, K. Optimization of squeeze cast process parameters on mechanical properties of Al₂O₃/SiC reinforced hybrid metal matrix composites using taguchi technique. In MATERIALS RESEARCH EXPRESS. ISSN 2053-1591, 2018, vol. 5, no. 6, pp., Registrované v: WOS

4. [1.1] RAHMAN, Md Obaidur - AHMAD, Saif Nawaz - PRIYADARSHI, Neeraj - SINGH, Raman Kumar - BHOI, Akash Kr. Processing and characterization of aluminium 2014-10Wt% SiC composite. In 2ND INTERNATIONAL CONFERENCE ON ADVANCES IN MECHANICAL ENGINEERING (ICAME 2018). ISSN 1757-8981, 2018, vol. 402, no., pp., Registrované v: WOS

ADCA300 PARCHOVIANSKÝ, Milan - GALUSEK, Dušan - ŠVANČÁREK, Peter - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Thermal behavior, electrical conductivity and microstructure of hot pressed Al₂O₃/SiC nanocomposites. In Ceramics International, 2014, vol. 40, no. 9, p. 14421-14429. (2013: 2.086 - IF, 0.812 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] EGELJA, Adela - PASALIC, Snezana - DODEVSKI, Vladimir - KRAGOVIC, Milan - STOJKOVIC-SIMATOVIC, Ivana - RADOVANOVIC, Zeljko - STOJMENOVIC, Marija. Structural, Morphological and Electrical Properties of Alumina/YAG Composites as Solid Electrolyte for IT SOFC. In SCIENCE OF SINTERING. ISSN 0350-820X, 2018, vol. 50, no. 3, pp. 357-369., Registrované v: WOS

2. [1.1] KUMAR, Sandeep - SARITA - NEHRA, Monika - DILBAGHI, Neeraj - TANKESHWAR, K. - KIM, Ki-Hyun. Recent advances and remaining challenges for polymeric nanocomposites in healthcare applications. In PROGRESS IN POLYMER SCIENCE. ISSN 0079-6700, 2018, vol. 80, no., pp. 1-38., Registrované v: WOS

ADCA301 PATEL, Niketan Sarabhai - PAVLÍK, Viliam - BOČA, Miroslav. High-temperature corrosion behavior of superalloys in molten salts - A review. In Critical Reviews in Solid State and Materials Sciences, 2017, vol. 42, no. 1, p. 83-97. (2016: 6.455 - IF, Q1 - JCR, 1.924 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 1040-8436.

Citácie:

1. [1.1] DING, Wenjin - BONK, Alexander - BAUER, Thomas. Corrosion behavior of metallic alloys in molten chloride salts for thermal energy storage in concentrated solar power plants: A review. In FRONTIERS OF CHEMICAL SCIENCE AND ENGINEERING. ISSN 2095-0179, 2018, vol. 12, no. 3, pp. 564-576., Registrované v: WOS

2. [1.1] GUO, Shaoqiang - WU, Evan - ZHANG, Jinsuo. Exchange current density of Gd(III)/Gd reaction in LiCl-KCl eutectic and analysis of errors caused by various methods. In ELECTROCHIMICA ACTA. ISSN 0013-4686, 2018, vol. 259, no., pp. 253-261., Registrované v: WOS

3. [1.1] HUANG, Hai - TANG, Xiaobin - CHEN, Feida - GAO, Fei - PENG, Qing - JI, Lulu - SUN, Xiangyu. Self-healing mechanism of irradiation defects in nickel-graphene nanocomposite: An energetic and kinetic perspective. In JOURNAL OF ALLOYS AND COMPOUNDS. ISSN 0925-8388, 2018, vol. 765, no., pp. 253-263., Registrované v: WOS

4. [1.1] KHORSAND, S. - SHEIKHI, A. - RAEISSI, K. - GOLOZAR, M. A. Hot Corrosion Behavior of Inconel 625 Superalloy in Eutectic Molten Nitrate Salts. In OXIDATION OF METALS. ISSN 0030-770X, 2018, vol. 90, no. 1-2, pp. 169-186., Registrované v: WOS

5. [1.1] QIU, Jie - LENG, Bin - LIU, Huajian - MACDONALD, Digby D. - WU, Angjian - JIA, Yanyan - XUE, Wandong - YU, Guojun - ZHOU, Xingtai. Effect of SO₂- on the corrosion of 316L stainless steel in molten FLiNaK salt. In CORROSION SCIENCE. ISSN 0010-938X, 2018, vol. 144, no., pp. 224-229., Registrované v: WOS

6. [1.1] REZAEI, Asma - KAMALI, Ali Reza. Green production of carbon nanomaterials in molten salts, mechanisms and applications. In DIAMOND AND RELATED MATERIALS. ISSN 0925-9635, 2018, vol. 83, no., pp. 146-161., Registrované v: WOS

ADCA302 PAVLÍK, Viliam - KONTRÍK, Martin - BOČA, Miroslav. Corrosion behavior of Incoloy 800H/HT in the fluoride molten salt FLiNaK + MF_x (MF_x = CrF₃, FeF₂, FeF₃ and NiF₂). In New Journal of Chemistry, 2015, vol. 39, no. 12, p. 9841-9847. (2014: 3.086 - IF, Q2 - JCR, 1.010 - SJR, Q1 - SJR,

karentované - CCC). (2015 - Current Contents). ISSN 1144-0546.

Citácie:

1. [1.1] AI, Hua - HOU, Juan - YE, Xiang-Xi - ZENG, Chao Liu - SUN, Hua - LI, Xiaoyun - YU, Guojun - ZHOU, Xingtai - WANG, Jian-Qiang. Influence of graphite-alloy interactions on corrosion of Ni-Mo-Cr alloy in molten fluorides. In *JOURNAL OF NUCLEAR MATERIALS*. ISSN 0022-3115, 2018, vol. 503, no., pp. 116-123., Registrované v: WOS
2. [1.1] DAI, Qilong - YE, Xiang-Xi - AI, Hua - CHEN, Shuangjian - JIANG, Li - LIANG, Jianping - YU, Kun - LENG, Bin - LI, Zhijun - ZHOU, Xingtai. Corrosion of Incoloy 800H alloys with nickel cladding in FLiNaK salts at 850 degrees C. In *CORROSION SCIENCE*. ISSN 0010-938X, 2018, vol. 133, no., pp. 349-357., Registrované v: WOS
3. [1.1] GUO, Shaoqiang - ZHANG, Jinsuo - WU, Wei - ZHOU, Wentao. Corrosion in the molten fluoride and chloride salts and materials development for nuclear applications. In *PROGRESS IN MATERIALS SCIENCE*. ISSN 0079-6425, 2018, vol. 97, no., pp. 448-487., Registrované v: WOS
4. [1.1] SARVGHAD, Madjid - MAHER, Salar Delkasar - COLLARD, David - TASSAN, Matthew - WILL, Geoffrey - STEINBERG, Theodore A. Materials compatibility for the next generation of Concentrated Solar Power plants. In *ENERGY STORAGE MATERIALS*. ISSN 2405-8297, 2018, vol. 14, no., pp. 179-198., Registrované v: WOS
5. [1.1] XUE, Wandong - YANG, Xinmei - YE, Xiang-Xi - HAN, Ling - WANG, Jianqiang - IGNATIEV, Victor - ZHOU, Xingtai. Effects of silicon carbide on the corrosion of metallic materials in molten LiF-NaF-KF salt. In *CORROSION SCIENCE*. ISSN 0010-938X, 2018, vol. 143, no., pp. 157-165., Registrované v: WOS
6. [1.1] ZHANG, Jinsuo - FORSBERG, Charles W. - SIMPSON, Michael F. - GUO, Shaoqiang - LAM, Stephen T. - SCARLAT, Raluca O. - CAROTTI, Francesco - CHAN, Kevin J. - SINGH, Preet M. - DONIGER, William - SRIDHARAN, Kumar - KEISER, James R. Redox potential control in molten salt systems for corrosion mitigation. In *CORROSION SCIENCE*. ISSN 0010-938X, 2018, vol. 144, no., pp. 44-53., Registrované v: WOS

ADCA303 PENTRÁK, Martin - MADEJOVÁ, Jana - KOMADEL, Peter. Effect of chemical composition and swelling on acid dissolution of 2:1 clay minerals. In *Philosophical Magazine*, 2010, vol. 90, no. 17-18, p. 2387-2397. (2009: 1.273 - IF, karentované - CCC). (2010 - Current Contents). ISSN 1478-6435.

Citácie:

1. [1.1] WANG, Qian - ZHU, Chang - YUN, Jiena - HU, Qiaoli - YANG, Gang. Compositional transformations as well as thermodynamics and mechanism of dissolution for clay minerals. In *CHEMICAL GEOLOGY*. ISSN 0009-2541, 2018, vol. 494, no., pp. 109-116., Registrované v: WOS

ADCA304 PENTRÁK, Martin - MADEJOVÁ, Jana - KOMADEL, Peter. Acid and alkali treatment of kaolins. In *Clay Minerals*, 2009, vol. 44, no. 4, p. 511-523. (2008: 0.500 - IF). ISSN 0009-8558.

Citácie:

1. [1.1] HUANG, Liuqin - FENG, Can - JIANG, Hongchen - DONG, Hailiang - LIU, Zizhang - ZENG, Qiang - WANG, Xi - ZHANG, Li. Reduction of structural Fe(III) in nontronite by thermophilic microbial consortia enriched from hot springs in Tengchong, Yunnan Province, China. In *CHEMICAL GEOLOGY*. ISSN 0009-2541, 2018, vol. 479, no., pp. 47-57., Registrované v: WOS
2. [1.1] WANG, Qian - ZHU, Chang - YUN, Jiena - HU, Qiaoli - YANG, Gang. Compositional transformations as well as thermodynamics and mechanism of dissolution for clay minerals. In *CHEMICAL GEOLOGY*. ISSN 0009-2541, 2018, vol. 494, no., pp. 109-116., Registrované v: WOS

ADCA305 PENTRÁK, Martin - BIZOVSKÁ, Valéria - MADEJOVÁ, Jana. Near-IR study of water adsorption on acid-treated montmorillonite. In *Vibrational Spectroscopy*, 2012, vol. 63, p. 360-366. (2011: 1.650 - IF, 0.608 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 0924-2031.

Citácie:

1. [1.1] BELHOCINE, M. - HAOUI, A. - BASSOU, G. - PHOU, T. - MAURIN, D. - BANTIGNIES, J. L. - HENN, F. Isosteric heat of water adsorption and desorption in homoionic alkaline-earth montmorillonites. In *CHEMICAL PHYSICS*. ISSN 0301-0104, 2018, vol. 501, no., pp. 26-34., Registrované v: WOS
2. [1.1] CAI, Jingong - DU, Jiazong - CHEN, Zewen - LEI, Tianzhu - ZHU, Xiaojun. HYDROTHERMAL EXPERIMENTS REVEAL THE INFLUENCE OF ORGANIC MATTER ON SMECTITE ILLITIZATION. In *CLAYS AND CLAY MINERALS*. ISSN 0009-8604, 2018, vol. 66, no. 1, pp. 28-42., Registrované v: WOS
3. [1.2] CHRYSSIKOS, G. D. Modern Infrared and Raman Instrumentation and Sampling Methods. In *Developments in Clay Science*. ISSN 15724352, 2017-01-01, 8, pp. 34-63., Registrované v: SCOPUS

ADCA306 PENTRÁK, Martin - CZÍMEROVÁ, Adriana - MADEJOVÁ, Jana - KOMADEL, Peter. Changes in layer charge of clay minerals upon acid treatment as obtained from their interactions with methylene blue. In *Applied Clay Science*, 2012, vol. 55, p. 100-107. (2011: 2.474 - IF, 1.165 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] BUJDAK, Juraj. The effects of layered nanoparticles and their properties on the molecular aggregation of organic dyes. In *JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY C-PHOTOCHEMISTRY REVIEWS*. ISSN 1389-5567, 2018, vol. 35, no., pp. 108-133., Registrované v: WOS
2. [1.1] DLUGOSZ, Olga - BANACH, Marcin. Kinetic, isotherm and thermodynamic investigations of the adsorption of Ag⁺ and Cu²⁺ on vermiculite. In *JOURNAL OF MOLECULAR LIQUIDS*. ISSN 0167-7322, 2018, vol. 258, no., pp. 295-309., Registrované v: WOS
3. [1.1] DONG, Jie - ZHANG, Junping. Biomimetic Super Anti-Wetting Coatings from Natural Materials Superamphiphobic Coatings Based on Nanoclays. In *SCIENTIFIC REPORTS*. ISSN 2045-2322, 2018, vol. 8, no., pp., Registrované v: WOS
4. [1.1] LI, Tingting - ZHAO, Lele - ZHENG, Ziliang - ZHANG, Min - SUN, Yidan - TIAN, Qingping - ZHANG, Shuqiu. Design and preparation acid-activated montmorillonite sustained-release drug delivery system for dexibuprofen in vitro and in vivo evaluations. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 163, no., pp. 178-185., Registrované v: WOS
5. [1.1] SONI, Vineet Kumar - ROY, Toran - DHARA, Suman - CHOUDHARY, Ganpat - SHARMA, Pragati R. - SHARMA, Rakesh

- K. On the investigation of acid and surfactant modification of natural clay for photocatalytic water remediation. In *JOURNAL OF MATERIALS SCIENCE*. ISSN 0022-2461, 2018, vol. 53, no. 14, pp. 10095-10110., Registrované v: WOS
6. [1.1] WĘGRZYN, Agnieszka - STAWINSKI, Wojciech - FREITAS, Olga - KOMEDERA, Kamila - BLACHOWSKI, Artur - JECZMIONEK, Lukasz - DANKO, Tomasz - MORDARSKI, Grzegorz - FIGUEIREDO, Sonia. Study of adsorptive materials obtained by wet fine milling and acid activation of vermiculite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 155, no., pp. 37-49., Registrované v: WOS
7. [1.2] CHERIFI-NACI, Halima. Synthesis and characterization of Ag-oxide pillar /composite clay mineral used as adsorbent. In *Research Journal of Chemistry and Environment*. ISSN 09720626, 2018-08-01, 22, 8, pp. 61-67., Registrované v: SCOPUS
- ADCA307 PERICHTA, P. - LIŠKA, Marek - MACHÁČEK, Jan - GEDEON, Ondrej. MD structural study of 23Y2O3-77Al2O3 and 23Al2O3-77Al2O3 glasses. In *Ceramics-Silikáty*, 2009, vol. 53, no. 1, p. 52-54. (2008: 0.644 - IF). ISSN 0862-5468.
- Citácie:
1. [1.1] ROSALES-SOSA, Gustavo A. - MASUNO, Atsunobu - HIGO, Yuji - WATANABE, Yasuhiro - INOUE, Hiroyuki. Effect of rare-earth ion size on elasticity and crack initiation in rare-earth aluminate glasses. In *JOURNAL OF THE AMERICAN CERAMIC SOCIETY*. ISSN 0002-7820, 2018, vol. 101, no. 11, pp. 5030-5036., Registrované v: WOS
- ADCA308 PETIT, Sabine - RIGHI, D. - MADEJOVÁ, Jana - DECARREAU, Alain. Layer charge estimation of smectites using infrared spectroscopy. In *Clay Minerals*, 1998, vol. 33, no. 4, p. 579-591. (1997: 0.640 - IF, karentované - CCC). (1998 - Current Contents). ISSN 0009-8558.
- Citácie:
1. [1.1] CHATTORAJ, Shovan L. - BANERJEE, Santanu - VAN DER MEER, Freek - RAY, P. K. Champati. Application of visible and infrared spectroscopy for the evaluation of evolved glauconite. In *INTERNATIONAL JOURNAL OF APPLIED EARTH OBSERVATION AND GEOINFORMATION*. ISSN 0303-2434, 2018, vol. 64, no., pp. 301-310., Registrované v: WOS
2. [1.1] EHLMANN, Bethany L. - HODYSS, Robert - BRISTOW, Thomas F. - ROSSMAN, George R. - AMMANNITO, Eleonora - DE SANCTIS, M. Cristina - RAYMOND, Carol A. Ambient and cold-temperature infrared spectra and XRD patterns of ammoniated phyllosilicates and carbonaceous chondrite meteorites relevant to Ceres and other solar system bodies. In *METEORITICS & PLANETARY SCIENCE*. ISSN 1086-9379, 2018, vol. 53, no. 9, pp. 1884-1901., Registrované v: WOS
3. [1.1] MISSANA, Tiziana - ALONSO, Ursula - MARIA FERNANDEZ, Ana - GARCIA-GUTIERREZ, Miguel. Colloidal properties of different smectite clays: Significance for the bentonite barrier erosion and radionuclide transport in radioactive waste repositories. In *APPLIED GEOCHEMISTRY*. ISSN 0883-2927, 2018, vol. 97, no., pp. 157-166., Registrované v: WOS
4. [1.1] SKIBA, Michal - SKIBA, Stefan - DERKOWSKI, Arkadiusz - MAJ-SZELIGA, Katarzyna - DZIUBINSKA, Beata. FORMATION OF NH4-ILLITE-LIKE PHASE AT THE EXPENSE OF DIOCTAHEDRAL VERMICULITE IN SOIL AND DIAGENETIC ENVIRONMENTS AN EXPERIMENTAL APPROACH. In *CLAYS AND CLAY MINERALS*. ISSN 0009-8604, 2018, vol. 66, no. 1, pp. 74-85., Registrované v: WOS
- ADCA309 PETIT, Sabine - RIGHI, D. - MADEJOVÁ, Jana. Infrared spectroscopy of NH4+ -bearing and saturated clay minerals: A review of the study of layer charge. In *Applied Clay Science*, 2006, vol. 34, no. 1-4, p. 22-30. (2005: 1.324 - IF, karentované - CCC). (2006 - Current Contents). ISSN 0169-1317.
- Citácie:
1. [1.1] JO, Jaeguk - YAMANAKA, Toshiro - KASHIMURA, Tomoki - OKUNISHI, Yusuke - KUWAHARA, Yoshihiro - KADOTA, Isao - MIYOSHI, Youko - ISHIBASHI, Jun-Ichiro - CHIBA, Hitoshi. Mineral nitrogen isotope signature in clay minerals formed under high ammonium environment conditions in sediment associated with ammonium-rich sediment-hosted hydrothermal system. In *GEOCHEMICAL JOURNAL*. ISSN 0016-7002, 2018, vol. 52, no. 4, pp. 317-333., Registrované v: WOS
2. [1.1] MROCZKOWSKA-SZERSZEN, Maja - ORZECOWSKI, Mateusz. Infrared spectroscopy methods in reservoir rocks analysis-semiquantitative approach for carbonate rocks. In *NAFTA-GAZ*. ISSN 0867-8871, 2018, vol. 74, no. 11, pp. 802-812., Registrované v: WOS
3. [1.1] RITZ, Michal - VALASKOVA, Marta. Infrared and Raman spectroscopy of three commercial vermiculites doped with cerium dioxide nanoparticles. In *SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY*. ISSN 1386-1425, 2018, vol. 201, no., pp. 39-45., Registrované v: WOS
4. [1.1] VAKALOVA, Tatyana - POGREBENKOV, Valeriy - VERESHAGIN, Vladimir - KHASBAS, Tamara - REVVA, Inna. Optimising rational chemical analysis for quantitative determination of the composition of clay in soils. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 163, no., pp. 153-163., Registrované v: WOS
- ADCA310 PETIT, Sabine - CAILLAUD, J. - RIGHI, D. - MADEJOVÁ, Jana - ELSASS, Francoise - KÖSTER, H.M. Characterization and crystal chemistry of an Fe-rich montmorillonite from Ölberg, Germany. In *Clay Minerals*, 2002, vol. 37, no. 2, p. 283-297. (2001: 0.610 - IF, karentované - CCC). (2002 - Current Contents). ISSN 0009-8558.
- Citácie:
1. [1.1] BODART, Philippe R. - DELMOTTE, L. - RIGOLET, S. - BRENDLE, J. - GOUGEON, Regis D. Li-7{F-19} TEDOR NMR to observe the lithium migration in heated montmorillonite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 157, no., pp. 204-211., Registrované v: WOS
2. [1.1] PELAYO, M. - MARCO, J. F. - FERNANDEZ, A. M. - VERGARA, L. - MELON, A. M. - PEREZ DEL VILLAR, L. Infrared and Mossbauer spectroscopy of Fe-rich smectites from Morron de Mateo bentonite deposit (Spain). In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 1, pp. 17-28., Registrované v: WOS
- ADCA311 PETIT, Sabine - MADEJOVÁ, Jana - DECARREAU, Alain - MARTIN, F. Characterization of octahedral substitutions in kaolinites using near infrared spectroscopy. In *Clays and Clay Minerals*, 1999, vol. 47, no. 1, p. 103-108. (1998: 1.010 - IF).
- Citácie:
1. [1.1] CHATTORAJ, Shovan L. - BANERJEE, Santanu - VAN DER MEER, Freek - RAY, P. K. Champati. Application of visible and infrared spectroscopy for the evaluation of evolved glauconite. In *INTERNATIONAL JOURNAL OF APPLIED EARTH OBSERVATION AND GEOINFORMATION*. ISSN 0303-2434, 2018, vol. 64, no., pp. 301-310., Registrované v: WOS

2. [1.1] DEGHFEL, Nadir - BENYAHIA, Azzedine - GUERFI, Kamel - ERRACHID, Abdelhamid - BELMOKRE, Kamel. Comparative study of the adsorption of a vat dye on different adsorbents based on an inorganic material Bentonite and clay from the M'sila region. In *MATERIAUX & TECHNIQUES*. ISSN 0032-6895, 2018, vol. 105, no. 4, pp., Registrované v: WOS
 3. [1.1] LAUKAMP, Carsten - WHITE, Alistair - RODGER, Andrew - GUM, Justin - METELKA, Vasek - LAU, Ian C. - GORDON, Georgina - FONTENEAU, Lionel C. MAPPING MINERAL FOOTPRINTS THROUGH COVER USING SURFACE AND SUBSURFACE MINERALOGY AND GEOCHEMISTRY. In *IGARSS 2018 2018 IEEE INTERNATIONAL GEOSCIENCE AND REMOTE SENSING SYMPOSIUM*. ISSN 2153-6996, 2018, vol., no., pp. 8352-8355., Registrované v: WOS
 4. [1.1] TSIANTOS, C. - GIONIS, V. - CHRYSSIKOS, G. D. Smectite in bentonite: Near infrared systematics and estimation of layer charge. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 160, no., pp. 81-87., Registrované v: WOS
 5. [1.1] YANG, Min - YE, Meifang - HAN, Haihui - REN, Guangli - HAN, Ling - ZHANG, Zhuan. Near-Infrared Spectroscopic Study of Chlorite Minerals. In *JOURNAL OF SPECTROSCOPY*. ISSN 2314-4920, 2018, vol., no., pp., Registrované v: WOS
- ADCA312 PETIT, Sabine - RIGHI, D. - MADEJOVÁ, Jana - DECARREAU, Alain. Interpretation of the infrared NH₄⁺ spectrum of the NH₄⁺-clays: application to the evaluation of the layer charge. In *Clay Minerals*, 1999, vol. 34, no. 4, p. 543-550. (1998: 1.130 - IF, karentované - CCC). (1999 - Current Contents).
- Citácie:
1. [1.1] ALAZIGHA, Dennis Pere - INDRARATNA, Buddhima - VINOD, Jayan S. - HEITOR, Ana. Mechanisms of stabilization of expansive soil with lignosulfonate admixture. In *TRANSPORTATION GEOTECHNICS*. ISSN 2214-3912, 2018, vol. 14, no., pp. 81-92., Registrované v: WOS
 2. [1.1] EHLMANN, Bethany L. - HODYSS, Robert - BRISTOW, Thomas F. - ROSSMAN, George R. - AMMANNITO, Eleonora - DE SANCTIS, M. Cristina - RAYMOND, Carol A. Ambient and cold-temperature infrared spectra and XRD patterns of ammoniated phyllosilicates and carbonaceous chondrite meteorites relevant to Ceres and other solar system bodies. In *METEORITICS & PLANETARY SCIENCE*. ISSN 1086-9379, 2018, vol. 53, no. 9, pp. 1884-1901., Registrované v: WOS
 3. [1.1] JO, Jaeguk - YAMANAKA, Toshiro - KASHIMURA, Tomoki - OKUNISHI, Yusuke - KUWAHARA, Yoshihiro - KADOTA, Isao - MIYOSHI, Youko - ISHIBASHI, Jun-Ichiro - CHIBA, Hitoshi. Mineral nitrogen isotope signature in clay minerals formed under high ammonium environment conditions in sediment associated with ammonium-rich sediment-hosted hydrothermal system. In *GEOCHEMICAL JOURNAL*. ISSN 0016-7002, 2018, vol. 52, no. 4, pp. 317-333., Registrované v: WOS
 4. [1.1] MINDRU, Ioana - GINGASU, Dana - DIAMANDESCU, Lucian - PATRON, Luminita - MARINESCU, Gabriela - CULITA, Daniela C. - CALDERON-MORENO, Jose Maria - PREDA, Silviu - OPREA, Ovidiu - PARVULESCU, Viorica. CoFe₂-xCr_xO₄ ferrites: synthesis, characterization and their catalytic activity. In *CHEMICAL PAPERS*. ISSN 2585-7290, 2018, vol. 72, no. 12, pp. 3203-3213., Registrované v: WOS
 5. [1.1] WU, Hanyu - QIANG, Shirong - FAN, Qiaohui - ZHAO, Xiaolan - LIU, Peng - LI, Ping - LIANG, Jianjun - WU, Wangsuo. Exploring the relationship between Th(IV) adsorption and the structure alteration of phlogopite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 152, no., pp. 295-302., Registrované v: WOS
- ADCA313 PETRA, Lukáš - BILLIK, Peter - MELICHOVÁ, Zuzana - KOMADEL, Peter. Mechanochemically activated saponite as materials for Cu²⁺ and Ni²⁺ removal from aqueous solutions. In *Applied Clay Science*, 2017, vol. 143, p. 22-28. (2016: 3.101 - IF, Q1 - JCR, 0.899 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0169-1317.
- Citácie:
1. [1.1] CHANTURIYA, Valentine A. - MINENKO, Vladimir G. - MAKAROV, Dmitriy V. - SUVOROVA, Olga V. - SELIVANOVA, Ekaterina A. Advanced Techniques of Saponite Recovery from Diamond Processing Plant Water and Areas of Saponite Application. In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 12., Registrované v: WOS
 2. [1.1] NEFZI, Houwaida - ABDERRABBA, Manef - AYADI, Sameh - LABIDI, Jalel. Formation of Palygorskite Clay from Treated Diatomite and its Application for the Removal of Heavy Metals from Aqueous Solution. In *WATER*. ISSN 2073-4441, 2018, vol. 10, no. 9., Registrované v: WOS
 3. [1.1] SAID, Ahmed - ZHANG, Qiwei - QU, Jun - LIU, Yanchu - LEI, Zhiwu - HU, Huimin - XU, Zhigao. Mechanochemical activation of phlogopite to directly produce slow-release potassium fertilizer. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 165, pp. 77-81., Registrované v: WOS
 4. [1.1] WEI, Guangtao - LI, Yunshang - ZHANG, Linye - CAI, Shuya - ZHU, Tong - LI, Zhongmin - MO, Jihua. Synthesis of bentonite-supported Fe(II) and heteropolyacid (HPW) composite through a mechanochemical processing. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 152, pp. 342-351., Registrované v: WOS
 5. [3.1] CHANTURIYA, V.A. - MINENKO, V.G. - MAKAROV, D.V. - SUVOROVA, O.V. - SELIVANOVA, E.A. Recycling Prospects for Saponite-Containing Water at Diamond Processing Plants in Arkhangelsk Region, Russia. In *PREPRINTS*. ISSN 2310-287X, 2018, 2018100463.
 6. [3.1] DOROSHENKO, D. - PYLYPENKO, I. - KORNILOVYCH, B. - SUBBOTA, I. Preparation of porous silica nanocomposites from montmorillonite using sol-gel approach. In *TECHNOLOGY AUDIT AND PRODUCTION RESERVES*. ISSN 2664-9969, 2018, vol. 4, no. 3, p. 42.
- ADCA314 PETRA, Lukáš - BILLIK, Peter - KOMADEL, Peter. Preparation and characterization of hybrid materials consisting of high-energy ground montmorillonite and α -amino acids. In *Applied Clay Science*, 2015, vol. 115, p. 174-178. (2014: 2.467 - IF, Q1 - JCR, 0.918 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0169-1317.
- Citácie:
1. [1.1] MERINO, D. - LUDUENA, L. N. - ALVAREZ, V. A. Dissimilar Tendencies of Innovative Green Clay Organo-Modifier on the Final Properties of Poly(ϵ -caprolactone) Based Nanocomposites. In *JOURNAL OF POLYMERS AND THE ENVIRONMENT*. ISSN 1566-2543, 2018, vol. 26, no. 2, pp. 716-727., Registrované v: WOS
 2. [1.1] SONI, Vineet Kumar - ROY, Toran - DHARA, Suman - CHOUDHARY, Ganpat - SHARMA, Pragati R. - SHARMA, Rakesh K. On the investigation of acid and surfactant modification of natural clay for photocatalytic water remediation. In *JOURNAL OF MATERIALS SCIENCE*. ISSN 0022-2461, 2018, vol. 53, no. 14, pp. 10095-10110., Registrované v: WOS
- ADCA315 PETRUŠKOVÁ, V. - VRÁBEL, Peter - ŠIMURKA, Peter - ŠAJGALÍK, Pavol - MARYŠKA, M.

Surface damage of two different wineglasses during dishwashing process. In *Ceramics-Silikáty*, 2007, vol. 51, no. 1, p. 57-66. (2006: 0.597 - IF, karentované - CCC). (2007 - Current Contents). ISSN 0862-5468.

Citácie:

1. [1.1] CERNA, Andrea - HRUSKA, Branislav - TOKARCIKOVA, Darinka - CHROMCIKOVA, Maria - LISKA, Marek. Optical microscopy, Raman spectroscopy, and AFM study of heavy weathered surface of barium crystal glass. In *CHEMICAL PAPERS*. ISSN 0366-6352, 2018, vol. 72, no. 9, pp. 2153-2158., Registrované v: WOS

2. [1.1] GURSES, M. Sadi - ERKEY, Can - KIZILEL, Seda - UZUN, Alper. Characterization of sodium tripolyphosphate and sodium citrate dehydrate residues on surfaces. In *TALANTA*. ISSN 0039-9140, 2018, vol. 176, no., pp. 8-16., Registrované v: WOS

ADCA316 PICHLBAUER, Sabine - HARMUTH, Harald - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol. Preliminary investigations of the production of MgAlON bonded refractories. In *Journal of the European Ceramic Society*, 2012, vol. 32, no. 9, p. 2013-2018. (2011: 2.353 - IF, 1.343 - SJR, karentované - CCC). (2012 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] YAN, Mingwei - LI, Yong - LI, Hongyu - SUN, Yang - CHEN, Haiyang - MA, Chenhong - SUN, Jialin. Evolution mechanism of MgAlON in the Al-Al₂O₃-MgO composite at 1800 degrees C in flowing nitrogen. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 4, pp. 3856-3861., Registrované v: WOS

ADCA317 PITONÁK, Michal - AQUILANTE, Francesco - HOBZA, Pavel - NEOGRÁDY, Pavel - NOGA, Jozef - URBAN, Miroslav. Parallelized implementation of the CCSD(T) method in MOLCAS using optimized virtual orbitals space and Cholesky decomposed two-electron integrals. In *Collection of Czechoslovak Chemical Communications*, 2011, vol. 76, no. 6, p. 713-742. (2010: 0.853 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0010-0765.

Citácie:

1. [1.1] NAGY, Peter R. - SAMU, Gyula - KALLAY, Mihaly. Optimization of the Linear-Scaling Local Natural Orbital CCSD(T) Method: Improved Algorithm and Benchmark Applications. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 8, pp. 4193-4215., Registrované v: WOS

ADCA318 PLACHKÝ, Tomáš - LENČEŠ, Zoltán - HRIC, Ľ. - ŠAJGALÍK, Pavol - BALÁŽ, Peter - RIEDEL, Ralf - KLEEBE, Hans-Joachim. Processing and mechanical properties of Si₃N₄ composites employing polymer-derived SiAlOC as sintering aid. In *Journal of the European Ceramic Society*, 2010, vol. 30, no. 3, p. 759-767. (2009: 2.090 - IF, karentované - CCC). (2010 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] BRINCKMANN, Stephan A. - PATRA, Niranjan - YAO, Jia - WARE, Taylor H. - FRICK, Carl P. - FERTIG, Ray S. Stereolithography of SiOC Polymer-Derived Ceramics Filled with SiC Micronwhiskers. In *ADVANCED ENGINEERING MATERIALS*. ISSN 1438-1656, 2018, vol. 20, no. 11, pp., Registrované v: WOS

2. [1.1] FIOCCO, Laura - AGNOLI, Stefano - PEDRON, Danilo - SECCO, Michele - TAMBURINI, Sergio - FERRONI, Letizia - GARDIN, Chiara - ZAVAN, Barbara - BERNARDO, Enrico. Wollastonite-diopside-carbon composite foams from a silicone resin and inorganic fillers. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 1, pp. 931-937., Registrované v: WOS

ADCA319 PRECNEROVÁ, Magdaléna - BODIŠOVÁ, Katarína - FRAJKOROVÁ, Františka - GALUSKOVÁ, Dagmar - VARCHULOVÁ NOVÁKOVÁ, Zuzana - VOJTAŠŠÁK, Ján - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol. In vitro bioactivity of silicon nitride-hydroxyapatite composites. In *Ceramics International*, 2015, vol. 41, no. 6, p. 8100-8108. (2014: 2.605 - IF, Q1 - JCR, 0.871 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] BOCK, Ryan M. - MARIN, Elia - RONDINELLA, Alfredo - BOSCHETTO, Francesco - ADACHI, Tetsuya - MCENTIRE, Bryan J. - BAL, B. Sonny - PEZZOTTI, Giuseppe. Development of a SiYAlON glaze for improved osteoconductivity of implantable medical devices. In *JOURNAL OF BIOMEDICAL MATERIALS RESEARCH PART B-APPLIED BIOMATERIALS*. ISSN 1552-4973, 2018, vol. 106, no. 3, pp. 1084-1096., Registrované v: WOS

2. [1.1] GUEDES-SILVA, Cecilia Chaves - DORION RODAS, Andrea Cecilia - SILVA, Antonio Carlos - RIBEIRO, Christiane - DE SOUZA CARVALHO, Flavio Machado - HIGA, Olga Zazuco - FERREIRA, Thiago dos Santos. Microstructure, Mechanical Properties and in vitro Biological Behavior of Silicon Nitride Ceramics. In *MATERIALS RESEARCH-IBERO-AMERICAN JOURNAL OF MATERIALS*. ISSN 1516-1439, 2018, vol. 21, no. 6, pp., Registrované v: WOS

ADCA320 PRNOVÁ, Anna - KLEMENT, Róbert - BODIŠOVÁ, Katarína - VALÚCHOVÁ, Jana - GALUSEK, Dušan - BRUNEEL, E. - VAN DRIESSCHE, I. Thermal behaviour of yttrium aluminate glasses studied by DSC, high-temperature X-ray diffraction, SEM and SEM-EDS. In *Journal of Thermal Analysis and Calorimetry*, 2017, vol. 128, no. 3, p. 1407-1415. (2016: 1.953 - IF, Q2 - JCR, 0.609 - SJR, Q2 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 1388-6150.

Citácie:

1. [1.1] MRAZEK, Jan - KASIK, Ivan - PROCHAZKOVA, Lenka - CUBA, Vaclav - GIRMAN, Vladimir - PUCHY, Viktor - BLANC, Wilfried - PETERKA, Pavel - AUBRECHT, Jan - CAJZL, Jakub - PODRAZKY, Ondrej. YAG Ceramic Nanocrystals Implementation into MCVD Technology of Active Optical Fibers. In *APPLIED SCIENCES-BASEL*. ISSN 2076-3417, 2018, vol. 8, no. 5, pp., Registrované v: WOS

ADCA321 PRNOVÁ, Anna - DOMANICKÁ, A. - KLEMENT, Róbert - KRAXNER, J. - POLOVKA, Martin - PENTRÁK, Martin - GALUSEK, Dušan - ŠIMURKA, Peter - KOZÁNKOVÁ, Jana. Er- and Nd-doped yttrium aluminosilicate glasses: Preparation and characterization. In *Optical Materials*, 2011, vol. 33, no. 12, p. 1872-1878. (2010: 1.678 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0925-

3467.

Citácie:

1. [1.1] LIFANTE, G. - MARTINEZ DE MENDIVIL, J. - HE, R. - CANTELAR, E. - ORTEGA SAN MARTIN, L. - SOLA, D. Transition probabilities of Er³⁺ ions in aluminosilicate glasses. In *JOURNAL OF LUMINESCENCE*. ISSN 0022-2313, 2018, vol. 203, no., pp. 305-312., Registrované v: WOS

2. [1.1] SHIH, Shao-Ju - CHOU, Yu-Jen - HADUSH, Abadi - LIN, Shih-Heng - HSIAO, Chih-Wei. Morphology Control of Eu-Doped Amorphous Gehlenite Phosphors Prepared by Spray Pyrolysis. In *JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY*. ISSN 1533-4880, 2018, vol. 18, no. 8, pp. 5849-5853., Registrované v: WOS

ADCA322 RAJAMÄKI, T. - KÁLLAY, M. - NOGA, Jozef - VALIRON, Pierre - HALONEN, L. High excitations in coupled-cluster series: vibrational energy levels of ammonia. In *Molecular Physics*, 2004, vol. 102, no. 21-22, p. 2297-2310.

Citácie:

1. [1.1] COLES, Phillip A. - OVSYANNIKOV, Roman I. - POLYANSKY, Oleg L. - YURCHENKO, Sergei N. - TENNYSON, Jonathan. Improved potential energy surface and spectral assignments for ammonia in the near-infrared region. In *JOURNAL OF QUANTITATIVE SPECTROSCOPY & RADIATIVE TRANSFER*. ISSN 0022-4073, 2018, vol. 219, no., pp. 199-212., Registrované v: WOS

ADCA323 RAKHMATULLIN, Aydar - POLOVOV, Ilya B. - MALTSEV, Dmitry - ALLIX, Mathieu - VOLKOVICH, Vladimir - CHUKIN, Andrey V. - BOČA, Miroslav - BESSADA, Catherine. Combined approach for the structural characterization of alkali fluoroscandates: Solid-state NMR, powder X-ray diffraction, and density functional theory calculations. In *Inorganic Chemistry*, 2018, vol. 57, no. 3, p. 1184-1195. (2017: 4.700 - IF, Q1 - JCR, 1.892 - SJR, Q1 - SJR, karentované - CCC). (2018 - Current Contents, WOS, SCOPUS). ISSN 0020-1669.

Citácie:

1. [1.1] CHEN, Daqin - PENG, Yongzhao - LI, Xinyue - ZHONG, Jiasong - HUAN, Ping. Competitive nanocrystallization of Na₃ScF₆ and NaYbF₄ in aluminosilicate glass and optical spectroscopy of Ln(3+) dopants. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 13, pp. 15666-15673., Registrované v: WOS

2. [1.1] SCHUBERT, Lea - DOERENKAMP, Carsten - HAVERKAMP, Sandra - HELETTA, Lukas - ECKERT, Hellmut - POETTGEN, Rainer. Sc₅Pd₄Si₆ crystal structure and Si-29/Sc-45 solid state MAS NMR spectroscopic investigations. In *DALTON TRANSACTIONS*. ISSN 1477-9226, 2018, vol. 47, no. 37, pp. 13025-13031., Registrované v: WOS

ADCA324 REGE, Pankaj D. - MALKINA, Oľga - GOROFF, Nancy S. The effect of Lewis bases on the ¹³C NMR of lodoalkynes. In *Journal of American Chemical Society*, 2002, vol. 124, no. 3, p. 370-371.

Citácie:

1. [1.1] DRAGHICI, Constantin - CAIRA, Mino R. - DUMITRESCU, Denisa E. - DUMITRASCU, Florea. Halogen Bonds of 4-Iodosydones in Solution Deduced from C-13-NMR Spectra. In *REVISTA DE CHIMIE*. ISSN 0034-7752, 2018, vol. 69, no. 4, pp. 843-845., Registrované v: WOS

2. [1.1] SZELL, Patrick M. J. - CAVALLO, Gabriella - TERRANEO, Giancarlo - METRANGOLO, Pierangelo - GABIDULLIN, Bulat - BRYCE, David L. Comparing the Halogen Bond to the Hydrogen Bond by Solid-State NMR Spectroscopy: Anion Coordinated Dimers from 2-and 3-Iodoethynylpyridine Salts. In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 44, pp. 11364-11376., Registrované v: WOS

3. [1.1] ZENG, Xiaobao - LIU, Chulong - YANG, Weiguang - WANG, Xingyong - WANG, Xinyan - HU, Yuefei. A general two-step one-pot synthesis process of ynones from alpha-keto acids and 1-iodoalkynes. In *CHEMICAL COMMUNICATIONS*. ISSN 1359-7345, 2018, vol. 54, no. 68, pp. 9517-9520., Registrované v: WOS

ADCA325 REPISKÝ, Michal - KOMOROVSKÝ, Stanislav - MALKIN, Elena - MALKINA, Oľga - MALKIN, Vladimír. Relativistic four-component calculations of electronic g-tensors in the matrix Dirac-Kohn-Sham framework. In *Chemical Physics Letters*, 2010, vol. 488, no. 1-3, p. 94-97. (2009: 2.291 - IF, karentované - CCC). (2010 - Current Contents). ISSN 0009-2614.

Citácie:

1. [1.1] PERSHINA, V. - ILIAS, M. Carbonyl compounds of Tc, Re, and Bh: Electronic structure, bonding, and volatility. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 20, pp., Registrované v: WOS

2. [1.1] SAYFUTYAROVA, Elvira R. - CHAN, Garnet Kin-Lic. Electron paramagnetic resonance g-tensors from state interaction spin-orbit coupling density matrix renormalization group. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 18, pp., Registrované v: WOS

3. [1.1] SCHATTENBERG, Caspar J. - MAIER, Toni M. - KAUPP, Martin. Lessons from the Spin-Polarization/Spin-Contamination Dilemma of Transition-Metal Hyperfine Couplings for the Construction of Exchange-Correlation Functionals. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 11, pp. 5653-5672., Registrované v: WOS

ADCA326 REPISKÝ, Michal - KOMOROVSKÝ, Stanislav - MALKINA, Oľga - MALKIN, Vladimír. Restricted magnetically balanced basis applied for relativistic calculations of indirect nuclear spin-spin coupling tensors in the matrix Dirac-Kohn-Sham framework. In *Chemical Physics*, 2009, vol. 356, no. 1-3, p. 236-242. (2008: 1.961 - IF, karentované - CCC). (2009 - Current Contents).

Citácie:

1. [1.1] RUSAKOVA, Irina L. - KRIVDIN, Leonid B. Relativistic effects in the NMR spectra of compounds containing heavy chalcogens. In *MENDELEEV COMMUNICATIONS*. ISSN 0959-9436, 2018, vol. 28, no. 1, pp. 1-13., Registrované v: WOS

ADCA327 REPISKÝ, Michal - KONEČNÝ, Lukáš - KÁDEK, Marius - KOMOROVSKÝ, Stanislav - MALKINA, Oľga - MALKIN, Vladimír - RUUD, Kenneth. Excitation energies from real-time propagation of the four-component Dirac-Kohn-Sham equation. In *Journal of Chemical Theory and Computation*, 2015, vol. 11, no. 3, p. 980-991. (2014: 5.498 - IF, Q1 - JCR, 2.803 - SJR, Q1 - SJR,

karentované - CCC). (2015 - Current Contents). ISSN 1549-9618.

Citácie:

1. [1.1] BANDYOPADHYAY, Arkamita - GHOSH, Dibyajyoti - PATI, Swapan K. *Shining Light on New-Generation Two-Dimensional Materials from a Computational Viewpoint*. In JOURNAL OF PHYSICAL CHEMISTRY LETTERS. ISSN 1948-7185, 2018, vol. 9, no. 7, pp. 1605-1612., Registrované v: WOS
2. [1.1] GOINGS, Joshua J. - EGIDI, Franco - LI, Xiaosong. *Current development of noncollinear electronic structure theory*. In INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY. ISSN 0020-7608, 2018, vol. 118, no. 1, pp., Registrované v: WOS
3. [1.1] GOINGS, Joshua J. - LESTRANGE, Patrick J. - LI, Xiaosong. *Real-time time-dependent electronic structure theory*. In WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE. ISSN 1759-0876, 2018, vol. 8, no. 1, pp., Registrované v: WOS
4. [1.1] LIAN, Chao - HU, Shi-Qi - GUAN, Meng-Xue - MENG, Sheng. *Momentum-resolved TDDFT algorithm in atomic basis for real time tracking of electronic excitation*. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 15, pp., Registrované v: WOS
5. [1.1] LIU, Wenjian - XIAO, Yunlong. *Relativistic time-dependent density functional theories*. In CHEMICAL SOCIETY REVIEWS. ISSN 0306-0012, 2018, vol. 47, no. 12, pp. 4481-4509., Registrované v: WOS
6. [1.1] MATTIAT, Johann - LUBER, Sandra. *Efficient calculation of (resonance) Raman spectra and excitation profiles with real-time propagation*. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 17, pp., Registrované v: WOS
7. [1.1] NORMAN, Patrick - DREUW, Andreas. *Simulating X-ray Spectroscopies and Calculating Core-Excited States of Molecules*. In CHEMICAL REVIEWS. ISSN 0009-2665, 2018, vol. 118, no. 15, pp. 7208-7248., Registrované v: WOS
8. [1.1] PETRONE, Alessio - WILLIAMS-YOUNG, David B. - SUN, Shichao - STETINA, Torin F. - LI, Xiaosong. *An efficient implementation of two-component relativistic density functional theory with torque-free auxiliary variables*. In EUROPEAN PHYSICAL JOURNAL B. ISSN 1434-6028, 2018, vol. 91, no. 7, pp., Registrované v: WOS
9. [1.1] REYNOLDS, Ryan D. - YANAI, Takeshi - SHIOZAKI, Toru. *Large-scale relativistic complete active space self-consistent field with robust convergence*. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 1, pp., Registrované v: WOS
10. [1.1] ROSSI, Tuomas P. - KUISMA, Mikael - PUSKA, Martti J. - NIEMINEN, Risto M. - ERHART, Paul. *Kohn-Sham Decomposition in Real-Time Time-Dependent Density-Functional Theory: An Efficient Tool for Analyzing Plasmonic Excitations*. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2017, vol. 13, no. 10, pp. 4779-4790., Registrované v: WOS
11. [1.1] SCHELTER, Ingo - KUEMMEL, Stephan. *Accurate Evaluation of Real-Time Density Functional Theory Providing Access to Challenging Electron Dynamics*. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 4, pp. 1910-1927., Registrované v: WOS
12. [1.1] SHIOZAKI, Toru. *An efficient solver for large structured eigenvalue problems in relativistic quantum chemistry*. In MOLECULAR PHYSICS. ISSN 0026-8976, 2017, vol. 115, no. 1-2, pp. 5-12., Registrované v: WOS
13. [1.1] SINHA-ROY, Rajarshi - GARCIA-GONZALEZ, Pablo - LOZANO, Xochitl Lopez - WHETTEN, Robert L. - WEISSKER, Hans-Christian. *Identifying Electronic Modes by Fourier Transform from delta-Kick Time-Evolution TDDFT Calculations*. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 12, pp. 6417-6426., Registrované v: WOS
14. [1.1] WU, Xiaojing - ALVAREZ-IBARRA, Aurelio - SALAHUB, Dennis R. - DE LA LANDE, Aurelien. *Retardation in electron dynamics simulations based on time-dependent density functional theory*. In EUROPEAN PHYSICAL JOURNAL D. ISSN 1434-6060, 2018, vol. 72, no. 12, pp., Registrované v: WOS

- ADCA328 RESCHKE, S. - HALUSCHKA, C. - RIEDEL, Ralf - LENČEŠ, Zoltán - GALUSEK, Dušan. *In situ generated homogeneous and functionally graded ceramic materials derived from polysilazane*. In Journal of the European Ceramic Society, 2003, vol. 23, no. 11, p. 1963-1970. ISSN 0955-2219.

Citácie:

1. [1.1] D'ELIA, Raffaele - DUSSERRE, Gilles - DEL CONFETTO, Sylvie - EBERLING-FUX, Nicolas - DESCAMPS, Cedric - CUTARD, Thierry. *Effect of dicumyl peroxide concentration on the polymerization kinetics of a polysilazane system*. In POLYMER ENGINEERING AND SCIENCE. ISSN 0032-3888, 2018, vol. 58, no. 6, pp. 859-869., Registrované v: WOS
2. [1.1] WANG, Qi - YANG, Mei - XIAO, Jiusan - JIAO, Shuqiang - ZHU, Hongmin. *Synthesis, characterization and sintering of Si-C-N nano-powders via sodium reduction in liquid ammonia*. In JOURNAL OF THE EUROPEAN CERAMIC SOCIETY. ISSN 0955-2219, 2018, vol. 38, no. 4, pp. 1219-1226., Registrované v: WOS

- ADCA329 REVIKINE, Roman - ARBUZNIKOV, Alexei V. - TREMBLAY, Jean-Christophe - REMENYI, Christian - MALKINA, Ol'ga - MALKIN, Vladimír - KAUPP, Martin. *Calculation of zero-field splitting parameters: Comparison of a two-component noncolinear spin-density-functional method and a one-component perturbational approach*. In Journal of Chemical Physics, 2006, vol. 125, no. 5, p. 054110-1-054110-12. (2005: 3.138 - IF). ISSN 0021-9606.

Citácie:

1. [1.1] BIKTAGIROV, Timur - SCHMIDT, Wolf Gero - GERSTMANN, Uwe. *Calculation of spin-spin zero-field splitting within periodic boundary conditions: Towards all-electron accuracy*. In PHYSICAL REVIEW B. ISSN 2469-9950, 2018, vol. 97, no. 11, pp., Registrované v: WOS

- ADCA330 RODE, B.M. - SON, H.L. - SUWANNACHOT, Y. - BUJDÁK, Juraj. *The combination of salt induced peptide formation reaction and clay catalysis: a way to higher peptides under primitive earth conditions*. In Origins of Life and Evolution of the Biosphere, 1999, vol. 29, no. 3, p. 273-286. (1998: 0.750 - IF).

Citácie:

1. [1.1] KITADAI, Norio - MARUYAMA, Shigenori. *Origins of building blocks of life: A review*. In GEOSCIENCE FRONTIERS. ISSN 1674-9871, 2018, vol. 9, no. 4, pp. 1117-1153., Registrované v: WOS

- ADCA331 SAHU, Sadananda - KAVECKÝ, Štefan - ILLÉSOVÁ, Ľubica - MADEJOVÁ, Jana - BERTÓTI, I. -

SZÉPVÖLGYI, János. Formation of boron nitride thin films on β -Si₃N₄ whiskers and α -SiC platelets by dip-coating. In *Journal of the European Ceramic Society*, 1998, vol. 18, no. 8, p.1037-1043. ISSN 0955-2219.

Citácie:

1. [1.1] LIU, Qiang - ZHAO, Bo - YANG, Chunping - ZHANG, Haoqian - ZHANG, Haijiao - ZHANG, Biao - YE, Feng - ZHOU, Yu. Fabrication of practically pure Si₂N₂O ceramic with high performance from amorphous BN surface modified nano-sized Si₃N₄ powders. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 1, pp. 333-337., Registrované v: WOS

2. [1.1] WU, Zhengtao - ZHONG, Xing - LIU, Cihai - WANG, Zhoucheng - DAI, Wei - WANG, Qimin. Plastic Deformation Induced by Nanoindentation Test Applied on ZrN/Si₃N₄ Multilayer Coatings. In *COATINGS*. ISSN 2079-6412, 2018, vol. 8, no. 1, pp., Registrované v: WOS

ADCA332 SALAMON, D. - SHEN, Zhijian - ŠAJGALÍK, Pavol. Rapid formation of alpha-sialon during spark plasma sintering: Its origin and implications. In *Journal of the European Ceramic Society*, 2007, vol. 27, no. 6, p. 2541-2547. (2006: 1.567 - IF, karentované - CCC). (2007 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] KHAN, Raja Muhammad Awais - AHMED, Bilal Anjum - AL MALKI, Moath Mohammad - HAKEEM, Abbas Saeed - LAOUI, Tahar. Synthesis of hard and tough calcium stabilized alpha-sialon/SiC ceramic composites using nano-sized precursors and spark plasma sintering. In *JOURNAL OF ALLOYS AND COMPOUNDS*. ISSN 0925-8388, 2018, vol. 757, no., pp. 200-208., Registrované v: WOS

2. [1.1] LERDPROM, Wirat - BHOWMIK, Ayan - GRASSO, Salvatore - ZAPATA-SOLVAS, Eugenio - JAYASEELAN, Doni D. - REECE, Michael J. - LEE, William E. Impact of spark plasma sintering (SPS) on mullite formation in porcelain. In *JOURNAL OF THE AMERICAN CERAMIC SOCIETY*. ISSN 0002-7820, 2018, vol. 101, no. 2, pp. 525-535., Registrované v: WOS

3. [1.1] ZUO, Fei - MENG, Fan - LIN, Dong-Tao - LV, Jian - YU, Jun-Jie - CHEN, Qiang - WANG, Hong-Jian - HE, Fu-Po - SENGGER, Marco - LIN, Hua-Tay. Effect of current pattern and conductive phase on sintering behavior of Si₃N₄-based ceramic composite. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 8, pp. 9561-9567., Registrované v: WOS

ADCA333 SAS, Samuel - DANKO, Martin - BIZOVSKÁ, Valéria - LANG, Kamil - BUJDÁK, Juraj. Highly luminescent hybrid materials based on smectites with polyethylene glycol modified with rhodamine fluorophore. In *Applied Clay Science*, 2017, vol. 138, p. 25-33. (2016: 3.101 - IF, Q1 - JCR, 0.899 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0169-1317.

Citácie:

1. [1.1] SHINDO, Yuta - INOSE, Tomoya - KUBOTA, Yohsuke - OIKAWA, Takahiro - TOKUNAGA, Masayuki - KAMEI, Takashi - GONDA, Kohsuke - KOBAYASHI, Yoshio. Synthesis on aggregation of colloidal solutions of ICG-active silica nanoparticles and their application in in-vivo fluorescence imaging. In *MATERIALS CHEMISTRY AND PHYSICS*. ISSN 0254-0584, 2018, vol. 220, no., pp. 201-207., Registrované v: WOS

ADCA334 SEDLÁČEK, Jaroslav - GALUSEK, Dušan - RIEDEL, Ralf - HOFFMANN, M.J. Sinter-HIP of polymer-derived Al₂O₃-SiC composites with high SiC contents. In *Materials Letters*, 2011, vol. 65, no. 15-16, p. 2462-2465. (2010: 2.117 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0167-577X.

Citácie:

1. [1.1] CAI, Yanzhi - CHENG, Laifei - YIN, Xiaowei - YIN, Hongfeng - WANG, Nan - ZHANG, Haijiao - WANG, Yuan. Effect of positioning impregnation on the oxidation behaviour of Ti₃SiC₂/SiC functionally graded materials at 1400 degrees C. In *JOURNAL OF ALLOYS AND COMPOUNDS*. ISSN 0925-8388, 2018, vol. 742, no., pp. 180-190., Registrované v: WOS

ADCA335 SEDLÁK, Richard - KOVALČÍKOVÁ, Alexandra - MÚDRA, Erika - RUTKOWSKI, Pawel - DUBIEL, Aleksandra - GIRMAN, Vladimír - BYSTRICKÝ, Roman - DUSZA, Ján. Boron carbide/graphene platelet ceramics with improved fracture toughness and electrical conductivity. In *Journal of the European Ceramic Society*, 2017, vol. 37, p. 3773-3780. (2016: 3.454 - IF, Q1 - JCR, 1.142 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0955-2219.

Citácie:

1. [1.1] ALEXANDER, Rajath - MURTHY, T. S. R. Ch. - VASANTHAKUMAR, K. - KARTHISELVA, N. S. - BAKSHI, Srinivasa Rao - DASGUPTA, Kinshuk. In-situ synthesis and densification of boron carbide and boron carbide-graphene nanoplatelet composite by reactive spark plasma sintering. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 17, pp. 21132-21137., Registrované v: WOS

2. [1.1] ALEXANDER, Rajath - MURTHY, T. S. R. Ch. - RAVIKANTH, K. V. - PRAKASH, Jyoti - MAHATA, Tarasankar - BAKSHI, Srinivasa Rao - KRISHNAN, Madangopal - DASGUPTA, Kinshuk. Effect of graphene nano-platelet reinforcement on the mechanical properties of hot pressed boron carbide based composite. In *Ceramics International*. ISSN 02728842, 2018-06-01, 44, 8, pp. 9830-9838., Registrované v: WOS

3. [1.1] CHENG, Chunyu - LI, Hejun - FU, Qiangang - GUO, Liping. Effect of Al₂O₃ on the densification and oxidation behavior of SiC coating for carbon/carbon composites. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 11, pp. 12702-12708., Registrované v: WOS

4. [1.1] LIU, Lixin - LI, Xuhai - HE, Qiang - XU, Liang - CAO, Xiuxia - PENG, Xusheng - MENG, Chuanmin - WANG, Wenqiang - ZHU, Wenjun - WANG, Yuan. Sintering dense boron carbide without grain growth under high pressure. In *JOURNAL OF THE AMERICAN CERAMIC SOCIETY*. ISSN 0002-7820, 2018, vol. 101, no. 3, pp. 1289-1297., Registrované v: WOS

5. [1.1] MURTHY, T. S. R. Ch. - ANKATA, Sairam - SONBER, J. K. - SAIRAM, K. - SINGH, Kulwant - NAGARAJ, A. - SENGUPTA, P. - BEDSE, R. D. - MAJUMDAR, Sanjib - KAIN, Vivekanand. MICROSTRUCTURE, THERMO-PHYSICAL, MECHANICAL AND WEAR PROPERTIES OF IN-SITU FORMED BORON CARBIDE ZIRCONIUM DIBORIDE COMPOSITE. In *CERAMICS-SILIKATY*. ISSN 0862-5468, 2018, vol. 62, no. 1, pp. 15-30., Registrované v: WOS

6. [1.1] RAMIREZ, Cristina - WANG, Qizhong - BELMONTE, Manuel - MIRANZO, Pilar - ISABEL OSENDI, M. - SHELDON, Brian W. - PADTURE, Nitin P. Direct in situ observation of toughening mechanisms in nanocomposites of silicon nitride and reduced graphene-oxide. In *SCRIPTA MATERIALIA*. ISSN 1359-6462, 2018, vol. 149, no., pp. 40-43., Registrované v: WOS
7. [1.1] SUN CHUAN - WAN CHUN-LEI - PAN WEI - ZONG PENG-AN - LI YUN-KAI - ZHOU SHI-MENG. Ballistic Performance of B₄C/Al₂O₃ Composite Ceramic Prepared by Reaction Sintering. In *JOURNAL OF INORGANIC MATERIALS*. ISSN 1000-324X, 2018, vol. 33, no. 5, pp. 545-549., Registrované v: WOS
8. [1.1] SUN, Guoxun - BI, Jianqiang - WANG, Weili - ZHANG, Jingde. Enhancing mechanical properties of fused silica composites by introducing well-dispersed boron nitride nanosheets. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 5, pp. 5002-5009., Registrované v: WOS
9. [1.1] THUMMARUNGSAN, Natlita - PARADEE, Nophawan - PATTAVARAKORN, Datchanee - SIRIVAT, Anuvat. Influence of graphene on electromechanical responses of plasticized poly(lactic acid). In *POLYMER*. ISSN 0032-3861, 2018, vol. 138, no., pp. 169-179., Registrované v: WOS

ADCA336 SHENDEROVICH, Ilja G. - SMIRNOV, S.N. - DENISOV, Gleb S. - GINDIN, V.A. - GOLUBEV, Nikolai S. - DUNGER, A. - REIBKE, R. - KIRPEKAR, S. - MALKINA, Oľga - LIMBACH, Hans-Heinrich. Nuclear magnetic resonance of hydrogen bonded clusters between F- and (HF)_n: Experiment and theory. In *Berichte der Bunsen-Gesellschaft - Physical Chemistry Chemical Physics*, 1998, vol. 102, no. 3, p. 422-428.

Citácie:

1. [1.1] DEAN, Natalie L. - MCINDOE, J. Scott. Fluoride-mediated rearrangement of phenylfluorosilanes. In *CANADIAN JOURNAL OF CHEMISTRY*. ISSN 0008-4042, 2018, vol. 96, no. 6, pp. 587-590., Registrované v: WOS
2. [1.1] MATSUNAMI, Asuka - KAYAKI, Yoshihito - KUWATA, Shigeki - IKARIYA, Takao. Nucleophilic Aromatic Substitution in Hydrodefluorination Exemplified by Hydrido-iridium(III) Complexes with Fluorinated Phenylsulfonyl-1,2-diphenylethylenediamine Ligands. In *ORGANOMETALLICS*. ISSN 0276-7333, 2018, vol. 37, no. 12, pp. 1958-1969., Registrované v: WOS
3. [1.1] ZHANG, Changzhe - LUO, Qi - CHENG, Shibo - BU, Yuxiang. Unusual Indirect Nuclear Spin-Spin Exchange Coupling through Solvated Electron. In *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*. ISSN 1948-7185, 2018, vol. 9, no. 4, pp. 689-695., Registrované v: WOS

ADCA337 SCHLEYER, P.V. - JIAO, H.J. - HOMMES, N.J.R.V. - MALKIN, Vladimír - MALKINA, Oľga. An evaluation of the aromaticity of inorganic rings: Refined evidence from magnetic properties. In *Journal of the American Chemical Society*, 1997, vol. 119, no. 51, p. 12669-12670. ISSN 0002-7863.

Citácie:

1. [1.1] AN, Ke - ZHU, Jun. Direct energetic evaluation of aromaticity by cleaving the rings of cyclic compounds. In *JOURNAL OF ORGANOMETALLIC CHEMISTRY*. ISSN 0022-328X, 2018, vol. 864, no., pp. 81-87., Registrované v: WOS
2. [1.1] BAEZ-GREZ, R. - RUIZ, Lina - PINO-RIOS, R. - TIZNADO, W. Which NICS method is most consistent with ring current analysis? Assessment in simple monocycles. In *RSC ADVANCES*. ISSN 2046-2069, 2018, vol. 8, no. 24, pp. 13446-13453., Registrované v: WOS
3. [1.1] COSTA, Alexandre - COSTA, Elizama Ramos - PEREIRA SILVA, Adilson Luis - TANAKA, Auro Atsushi - GOMES VARELA JUNIOR, Jaldyr de Jesus. Theoretical study of the effects of substituents (F, Cl, Br, CH₃, and CN) on the aromaticity of borazine. In *JOURNAL OF MOLECULAR MODELING*. ISSN 1610-2940, 2018, vol. 24, no. 1, pp., Registrované v: WOS
4. [1.1] DEMPSEY, Katie - MIR, Roya - SMAJLAGIC, Ivor - DUDDING, Travis. Expanding the repertoire of cyclopropenium ion phase transfer catalysis: Benzylic fluorination. In *TETRAHEDRON*. ISSN 0040-4020, 2018, vol. 74, no. 27, pp. 3507-3511., Registrované v: WOS
5. [1.1] DRIVER, Nicholas - JENA, Purusottam. Electron affinity of modified benzene. In *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY*. ISSN 0020-7608, 2018, vol. 118, no. 4, pp., Registrované v: WOS
6. [1.1] FIZER, Maksym - SLIVKA, Mikhailo - MARIYCHUK, Ruslan - BAUMER, Vjacheslav - LENDEL, Vasil. 3-Methylthio-4-phenyl-5-phenylamino-1,2,4-triazole hexabromotellurate: X-ray and computational study. In *JOURNAL OF MOLECULAR STRUCTURE*. ISSN 0022-2860, 2018, vol. 1161, no., pp. 226-236., Registrované v: WOS
7. [1.1] GESSNER, Viktoria H. Reactivity and Applications of alpha-Metalated Ylides. In *MODERN YLIDE CHEMISTRY: APPLICATIONS IN LIGAND DESIGN, ORGANIC AND CATALYTIC TRANSFORMATIONS*. ISSN 0081-5993, 2018, vol. 177, no., pp. 117-155., Registrované v: WOS
8. [1.1] HERMANN, Mathias - WASSY, Daniel - KRATZERT, Daniel - ESSER, Birgit. Dibenzo[a,e]pentalenophanes: Bending a Non-Alternant Hydrocarbon. In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 29, pp. 7374-+, Registrované v: WOS
9. [1.1] JENA, Puru - SUN, Qiang. Super Atomic Clusters: Design Rules and Potential for Building Blocks of Materials. In *CHEMICAL REVIEWS*. ISSN 0009-2665, 2018, vol. 118, no. 11, pp. 5755-5870., Registrované v: WOS
10. [1.1] KALEMOS, Apostolos. The nature of the chemical bond in borazine (B₃N₃H₆), boroxine (B₃O₃H₃), carborazine (B₂N₂C₂H₆), and related species. In *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY*. ISSN 0020-7608, 2018, vol. 118, no. 16, pp., Registrované v: WOS
11. [1.1] KARADAKOV, Peter B. - AL-YASSIRI, Muntadar A. H. - COOPER, David L. Magnetic Shielding, Aromaticity, Antiaromaticity and Bonding in the Low-Lying Electronic States of S₂N₂. In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 63, pp. 16791-16803., Registrované v: WOS
12. [1.1] KOOHI, Maryam - SOLEIMANI-AMIRI, Somayeh - SHARIATI, Minoo. Novel X- and Y-substituted heterofullerenes X₄Y₄C₁₂ developed from the nanocage C-20, where X = B, Al, Ga, Si and Y = N, P, As, Ge: a comparative investigation on their structural, stability, and electronic properties at DFT. In *STRUCTURAL CHEMISTRY*. ISSN 1040-0400, 2018, vol. 29, no. 3, pp. 909-920., Registrované v: WOS
13. [1.1] LI, Qing - XU, Hong-Liang - SU, Zhong-Min. NICS values scan in three-dimensional space of the hoop-shaped pi-conjugated molecules [6](8)cyclacene and [16]trannulene. In *NEW JOURNAL OF CHEMISTRY*. ISSN 1144-0546, 2018, vol. 42, no. 3, pp. 1987-1994., Registrované v: WOS
14. [1.1] LU, Sheng-Jie - WU, Li-Shun - LIN, Feng. Probing the geometric structures and bonding mechanisms of Cu-I hybrid clusters: Cu₄I₄-0. In *COMPUTATIONAL AND THEORETICAL CHEMISTRY*. ISSN 2210-271X, 2018, vol. 1139, no., pp. 102-

105., Registrované v: WOS

15. [1.1] LU, Sheng-Jie - WU, Li-Shun - LIN, Feng. Probing the geometric structures and bonding properties in Nb₂Si₂O (-/0) clusters by density functional theory calculations. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 709, no., pp. 60-64., Registrované v: WOS

16. [1.1] LU, Sheng-Jie - WU, Li-Shun - LIN, Feng. Probing the structures and properties of Ti₂Si₂O/-0 clusters by density functional theory calculations. In *CHEMICAL PHYSICS LETTERS*. ISSN 0009-2614, 2018, vol. 707, no., pp. 108-112., Registrované v: WOS

17. [1.1] LU, Sheng-Jie - XU, Xi-Ling - XU, Hong-Guang - ZHENG, Wei-Jun. Structural evolution and bonding properties of Au₂Si_n-0 (n=1-7) clusters: Anion photoelectron spectroscopy and theoretical calculations. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 24, pp., Registrované v: WOS

18. [1.1] MIRZA, Behrooz - SOLEIMANI-AMIRI, Somayeh - MIRZA, Maziar. Reaching for [6](n) SiC-cyclacenes and [6](n) SiC-acenes: A DFT approach. In *JOURNAL OF PHYSICAL ORGANIC CHEMISTRY*. ISSN 0894-3230, 2018, vol. 31, no. 2, pp., Registrované v: WOS

19. [1.1] NOROOZI-SHAD, Nazanin - GHOLIZADEH, Mostafa - IZADYAR, Mohammad. Direct C2-arylation of quinoline N-oxides by boronic esters; a molecular approach on the efficient metal-free method in C-C cross-coupling reactions. In *RESEARCH ON CHEMICAL INTERMEDIATES*. ISSN 0922-6168, 2018, vol. 44, no. 1, pp. 657-673., Registrované v: WOS

20. [1.1] PARKE, Sarah M. - NARRETO, Mary A. B. - HUPF, Emanuel - MCDONALD, Robert - FERGUSON, Michael J. - HEGMANN, Frank A. - RIVARD, Eric. Understanding the Origin of Phosphorescence in Bismoles: A Synthetic and Computational Study. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 13, pp. 7536-7549., Registrované v: WOS

21. [1.1] PENG, Hongliang - HUANG, Pengru - YI, Pinggui - XU, Fen - SUN, Lixian. Theoretical studies of pi-electron delocalization and localization on intramolecular proton transfer in the ground state. In *JOURNAL OF MOLECULAR STRUCTURE*. ISSN 0022-2860, 2018, vol. 1154, no., pp. 590-595., Registrované v: WOS

22. [1.1] SHEN, Chen-fei - LIU, Zi-zhong - LIU, Hong-xia - ZHANG, Hui-qing. Bond Length Equalization with molecular aromaticity-A new measurement of aromaticity. In *SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY*. ISSN 1386-1425, 2018, vol. 201, no., pp. 392-398., Registrované v: WOS

23. [1.1] SOLEIMANI-AMIRI, Somayeh - KOOHI, Maryam - AZIZI, Zahra. Characterization of nonsegregated C₁₇Si₃ heterofullerene isomers using density functional theory method. In *JOURNAL OF THE CHINESE CHEMICAL SOCIETY*. ISSN 0009-4536, 2018, vol. 65, no. 12, pp. 1453-1464., Registrované v: WOS

24. [1.1] SOURI, Maryam - MOHAMMADI, Kobra. Theoretical investigation of the defect position effect on the NLO properties of N and B doped graphenes. In *JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY*. ISSN 1010-6030, 2018, vol. 367, no., pp. 39-44., Registrované v: WOS

25. [1.1] TUPIKINA, Elena Yu. - EFIMOVA, Alexandra A. - DENISOV, Gleb S. - TOLSTOY, Peter M. Outer electronic shell visualization by NMR chemical shift laplacian of a helium probe. In *JOURNAL OF COMPUTATIONAL CHEMISTRY*. ISSN 0192-8651, 2018, vol. 39, no. 29, pp. 2459-2462., Registrované v: WOS

26. [1.1] VAN DE WOUW, Heidi L. - AWUYAH, Elorm C. - BARIS, Jodie I. - KLAUSEN, Rebekka S. An Organoborane Vinyl Monomer with Styrene-like Radical Reactivity: Reactivity Ratios and Role of Aromaticity. In *MACROMOLECULES*. ISSN 0024-9297, 2018, vol. 51, no. 16, pp. 6359-6368., Registrované v: WOS

27. [1.1] VERMA, Kanupriya - VISWANATHAN, K. S. "A Tale of Two Structures": The Stacks and Ts of Borazine and Benzene Hetero and Homo Dimers. In *CHEMISTRYSELECT*. ISSN 2365-6549, 2018, vol. 3, no. 3, pp. 864-873., Registrované v: WOS

28. [1.1] WEN, Mei - LI, Zhuo Zhe - LI, An Yong. Noble gas inserted compounds of borazine and its derivative B₃N₃R₆: structures and bonding. In *JOURNAL OF MOLECULAR MODELING*. ISSN 1610-2940, 2018, vol. 24, no. 11, pp., Registrované v: WOS

29. [1.1] XIE, Xiao-Hua - ZHAO, Xin-Wei - LI, Ming. Theoretical Study on the Photoelectric Properties of a Class of Copolymers Based on Benzodithiophene for Solar Cells. In *INTERNATIONAL JOURNAL OF POLYMER SCIENCE*. ISSN 1687-9422, 2018, vol., no., pp., Registrované v: WOS

30. [1.1] XIE, Xiaohua - FENG, Xianghua - ZHAO, Xinwei. The effects of electronic structures of four benzodithiophene-based copolymers on their photovoltaic performances. In *COMPUTATIONAL AND THEORETICAL CHEMISTRY*. ISSN 2210-271X, 2018, vol. 1145, no., pp. 28-36., Registrované v: WOS

31. [1.1] XU, Xi-Ling - YANG, Bin - WEI, Zhi-You - CAO, Guo-Jin - XU, Hong-Guang - ZHENG, Wei-Jun. Structural and bonding properties of Cu₃O₃- and Cu₃O₄- clusters: anion photoelectron spectroscopy and density functional calculations. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 31, pp. 20622-20628., Registrované v: WOS

32. [1.1] YEOLE, Sachin D. - KHIRE, Subodh S. - SARODE, Chandrakant H. - PATIL, Kadu D. On the cation-pi interactions in 1,2-dihydro-1,2-azaborine. In *JOURNAL OF CHEMICAL SCIENCES*. ISSN 0974-3626, 2018, vol. 130, no. 8, pp., Registrované v: WOS

33. [1.1] ZHANG, Xinxing - LUNDELL, Katie A. - OLSON, Jared K. - BOWEN, Kit H. - BOLDYREV, Alexander I. Electronic Transmutation (ET): Chemically Turning One Element into Another. In *CHEMISTRY-A EUROPEAN JOURNAL*. ISSN 0947-6539, 2018, vol. 24, no. 37, pp. 9200-9210., Registrované v: WOS

34. [1.1] ZHAO, Xue-Feng - LI, Jia-Jia - LI, Hai-Ru - YUAN, Caixia - TIAN, Xinxin - LI, Si-Dian - WU, Yan-Bo - GUO, Jin-Chang - WANG, Zhi-Xiang. Viable aromatic BenHn stars enclosing a planar hypercoordinate boron or late transition metal. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 10, pp. 7217-7222., Registrované v: WOS

ADCA338 SCHOLTZOVA, Eva - MADEJOVA, Jana - JANKOVIC, Luboš - TUNEGA, Daniel. Structural and spectroscopic characterization of montmorillonite intercalated with N-butylammonium cations (N = 1-4) - modeling and experimental study. In *Clays and Clay Minerals*, 2016, vol. 64, no. 4, p. 401-412. (2015: 1.222 - IF, Q3 - JCR, 0.504 - SJR, Q2 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0009-8604.

Citácie:

1. [1.1] CHURAKOV, Sergey V. - LIU, Xiandong. Quantum-chemical modelling of clay mineral surfaces and clay mineral-surface-adsorbate interactions. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9*. ISSN 1572-4352, 2018, vol. 9, no., pp. 49-87., Registrované v: WOS

2. [1.1] WEI, Yanke - MEI, Lefu - LI, Rui - LIU, Meng - LV, Guocheng - WENG, Jianle - LIAO, Libing - LI, Zhaohui - LU, Lin. Fabrication of an AMC/MMT Fluorescence Composite for its Detection of Cr(VI) in Water. In *FRONTIERS IN CHEMISTRY*. ISSN 2296-2646, 2018, vol. 6, no., pp., Registrované v: WOS

ADCA339 SCHOLTZO VÁ, Eva - TUNEGA, Daniel - SPEZIALE, S. Mechanical properties of ettringite and thaumasite - DFT and experimental study. In *Cement and Concrete Research*, 2015, vol. 77, p. 9-15. (2014: 2.864 - IF, Q1 - JCR, 4.201 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0008-8846.

Citácie:

1. [1.1] SAN, Saro - LI, Neng - TAO, Yong - ZHANG, Wenqin - CHING, Wai-Yim. Understanding the atomic and electronic origin of mechanical property in thaumasite and ettringite mineral crystals. In *JOURNAL OF THE AMERICAN CERAMIC SOCIETY*. ISSN 0002-7820, 2018, vol. 101, no. 11, pp. 5177-5187., Registrované v: WOS

2. [1.1] ZAJAC, Maciej - SKOCEK, Jan - ADU-AMANKWAH, Samuel - BLACK, Leon - BEN HAHA, Mohsen. Impact of microstructure on the performance of composite cements: Why higher total porosity can result in higher strength. In *CEMENT & CONCRETE COMPOSITES*. ISSN 0958-9465, 2018, vol. 90, no., pp. 178-192., Registrované v: WOS

ADCA340 SCHOLTZO VÁ, Eva - KUCKOVÁ, Lenka - KOŽÍŠEK, Jozef - TUNEGA, Daniel. Structural and spectroscopic characterization of ettringite mineral - combined DFT and experimental study. In *Journal of Molecular Structure*, 2015, vol. 1100, p. 215-224. (2014: 1.602 - IF, Q3 - JCR, 0.442 - SJR, Q3 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 0022-2860.

Citácie:

1. [1.1] SAN, Saro - LI, Neng - TAO, Yong - ZHANG, Wenqin - CHING, Wai-Yim. Understanding the atomic and electronic origin of mechanical property in thaumasite and ettringite mineral crystals. In *JOURNAL OF THE AMERICAN CERAMIC SOCIETY*. ISSN 0002-7820, 2018, vol. 101, no. 11, pp. 5177-5187., Registrované v: WOS

2. [1.1] ZHANG DING-WEN - XIANG LIAN - CAO ZHI-GUO. Effect of CaO on ettringite stabilization/solidification of lead-contaminated soil. In *ROCK AND SOIL MECHANICS*. ISSN 1000-7598, 2018, vol. 39, no. 1, pp. 29-35., Registrované v: WOS

ADCA341 SCHOLTZO VÁ, Eva - TURI NAGY, L. - PUTYERA, Karol. Modeling of nontraditional structures of carbon. In *Journal of chemical information and computer sciences*. - Washington : American Chemical Society, 2001, vol. 41, no. 1, p. 451-456. ISSN 0095-2338.

Citácie:

1. [1.1] HU, Meng - DONG, Xiao - WU, Yingju - LIU, Lingyu - ZHAO, Zhisheng - ZHOU, Xiang-Feng - STROBEL, Timothy A. - GAO, Guoying - TIAN, Yongjun - HE, Julong. Low-energy 3D sp(2) carbons with versatile properties beyond graphite and graphene. In *DALTON TRANSACTIONS*. ISSN 1477-9226, 2018, vol. 47, no. 17, pp. 6233-6239., Registrované v: WOS

ADCA342 SCHOLTZO VÁ, Eva - BENCO, Ľubomír - TUNEGA, Daniel. A model study of dickite intercalated with formamide and N-methylformamide. In *Physics and chemistry of minerals*, 2008, vol. 35, no. 6, p. 299-309. (2008 - Current Contents). ISSN 0342-1791.

Citácie:

1. [1.1] WANG, Guanshi - LAI, Yuanming - PENG, Chenliang. Adsorption of rare earth yttrium and ammonium ions on kaolinite surfaces: a DFT study. In *THEORETICAL CHEMISTRY ACCOUNTS*. ISSN 1432-881X, 2018, vol. 137, no. 4, pp., Registrované v: WOS

2. [1.1] ZHANG, Shuai - LIU, Qinfu - GAO, Feng - MA, Rujia - WU, Zeguang - TEPPEN, Brian J. Interfacial structure and interaction of kaolinite intercalated with N-methylformamide insight from molecular dynamics modeling. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 158, no., pp. 204-210., Registrované v: WOS

3. [1.1] ZHANG, Shuai - LIU, Qinfu - GAO, Feng - TEPPEN, Brian J. Molecular Dynamics Simulation of Basal Spacing, Energetics, and Structure Evolution of a Kaolinite-Formamide Intercalation Complex and Their Interfacial Interaction. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 6, pp. 3341-3349., Registrované v: WOS

4. [1.1] ZHONG XIANG-HUA - LIU YU - LIU WEN-YUAN - XU TAO. Preparation and Mechanism of Dickite-cesium Acetate Intercalated Complex. In *CAILIAO GONGCHENG-JOURNAL OF MATERIALS ENGINEERING*. ISSN 1001-4381, 2018, vol. 46, no. 7, pp. 76-82., Registrované v: WOS

5. [1.1] ZHONG, Xiang-Hua - LIU, Yu - XU, Tao - LIU, Wen-Yuan. Influencing factors of intercalation of potassium acetate into dickite using immersion method. In *JOURNAL OF ALLOYS AND COMPOUNDS*. ISSN 0925-8388, 2018, vol. 742, no., pp. 996-1001., Registrované v: WOS

ADCA343 SCHOLTZO VÁ, Eva - TUNEGA, Daniel - TURI NAGY, L. Theoretical study of cation substitution in trioctahedral sheet of phyllosilicates. An effect on inner OH group. In *Journal of Molecular Structure*. Thechem, 2003, vol. 620, no. 1, p. 1-8. ISSN 0166-1280.

Citácie:

1. [1.1] BOBICKI, Erin R. - LIU, Qingxia - XU, Zhenghe. Microwave Treatment of Ultramafic Nickel Ores: Heating Behavior, Mineralogy, and Comminution Effects. In *MINERALS*. ISSN 2075-163X, 2018, vol. 8, no. 11, pp., Registrované v: WOS

2. [1.1] NAYANTHIKA, I. V. K. - JAYAWARDANA, D. T. - BANDARA, N. J. G. J. - MANAGE, P. M. - MADUSHANKA, R. M. T. D. Effective use of iron-aluminum rich laterite based soil mixture for treatment of landfill leachate. In *WASTE MANAGEMENT*. ISSN 0956-053X, 2018, vol. 74, no., pp. 347-361., Registrované v: WOS

ADCA344 SCHOLTZO VÁ, Eva - TUNEGA, Daniel - MADEJO VÁ, Jana - PÁLKOVÁ, Helena - KOMADEL, Peter. Theoretical and experimental study of montmorillonite intercalated with tetramethylammonium cation. In *Vibrational Spectroscopy*, 2013, vol. 66, p. 123-131. (2012: 1.747 - IF, 0.549 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 0924-2031.(APVV-0362-10 : Organoily a ich kompozity s polymérmi. APVV SK-AT-0020-10 : Molekulové simulácie vybraných organoílov - charakterizácia štruktúry a vlastností).

Citácie:

1. [1.1] ROBLES, Irma - BANDALA, Yamir - MANRIQUEZ, Juan - BUSTOS, Erika. Modeling of Hg (II) Adsorption onto Ca-

- bentonite. In *JOURNAL OF THE MEXICAN CHEMICAL SOCIETY*. ISSN 1870-249X, 2018, vol. 62, no. 2, pp. 305-313., Registrované v: WOS
2. [1.1] YANG, Zongyi - LIU, Wenli - ZHANG, He - JIANG, Xinli - MIN, Fanfei. DFT study of the adsorption of 3-chloro-2-hydroxypropyl trimethylammonium chloride on montmorillonite surfaces in solution. In *APPLIED SURFACE SCIENCE*. ISSN 0169-4332, 2018, vol. 436, no., pp. 58-65., Registrované v: WOS
3. [1.2] TOTURBIEV, B. D. - TOTURBIEV, A. B. - ABDULLAEV, M. Sh - ABDULGANIEVA, T. I. Use of clay rocks in expanded clay aggregate production. In *Gornyi Zhurnal*. ISSN 00172278, 2018-03-01, 3, pp. 58-62., Registrované v: SCOPUS
4. [1.2] YANG, Zongyi - LIU, Wenli - ZHAO, Rao - CHEN, Jianhua. DFT study on the inhibition of hydration expansion of montmorillonite by 2-hydroxyethyl trimethyl ammonium chloride. In *Meitan Xuebao/Journal of the China Coal Society*. ISSN 02539993, 2018-03-01, 43, 3, pp. 831-838., Registrované v: SCOPUS
- ADCA345 SINGH, Meinam Annebushan - SARMA, Deba Kumar - HANZEL, Ondrej - SEDLÁČEK, Jaroslav - ŠAJGALÍK, Pavol. Machinability analysis of multi walled carbon nanotubes filled alumina composites in wire electrical discharge machining process. In *Journal of the European Ceramic Society*, 2017, vol. 37, no. 9, p. 3107-3114. (2016: 3.454 - IF, Q1 - JCR, 1.142 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0955-2219.
- Citácie:
1. [1.1] WANG, Jin - FU, Cheng - JIA, Zhixin. Cutting of hard and brittle insulating materials using spark discharge-assisted diamond wire sawing. In *JOURNAL OF MATERIALS PROCESSING TECHNOLOGY*. ISSN 0924-0136, 2018, vol. 252, no., pp. 225-232., Registrované v: WOS
2. [1.1] WANG, Jin - GUO, Y. B. - FU, Cheng - JIA, Zhixin. Surface integrity of alumina machined by electrochemical discharge assisted diamond wire sawing. In *JOURNAL OF MANUFACTURING PROCESSES*. ISSN 1526-6125, 2018, vol. 31, no., pp. 96-102., Registrované v: WOS
- ADCA346 SKLENÁK, Štěpán - ANDRIKOPOULOS, Prokopis C. - WHITTLETON, Sarah R. - JIRGLOVÁ, Hana - SAZAMA, Petr - BENCO, Ľubomír - BUČKO, Tomáš - HAFNER, Jürgen - SOBALÍK, Zdeněk. Effect of the Al siting on the structure of Co(II) and Cu(II) cationic sites in ferrierite. A periodic DFT molecular dynamics and FTIR study. In *Journal of Physical Chemistry C*, 2013, vol. 117, no. 8, p. 3958-3968. (2012: 4.814 - IF, 2.514 - SJR, karentované - CCC). (2013 - Current Contents, WOS, SCOPUS). ISSN 1932-7447.
- Citácie:
1. [1.1] KNOTT, Brandon C. - NIMLOS, Claire T. - ROBICHAUD, David J. - NIMLOS, Mark R. - KIM, Seonah - GOUNDER, Rajamani. Consideration of the Aluminum Distribution in Zeolites in Theoretical and Experimental Catalysis Research. In *ACS CATALYSIS*. ISSN 2155-5435, 2018, vol. 8, no. 2, pp. 770-784., Registrované v: WOS
- ADCA347 SLOSIARIKOVÁ, Hana - BUJDÁK, Juraj - HLAVATÝ, V. IR-spectra of octadecylammonium-montmorillonite in the range of the Si-O vibrations. In *Journal of Inclusion Phenomena and Molecular Recognition in Chemistry*, 1992, vol. 13, no. 3, p. 267-272.
- Citácie:
1. [1.1] CHEN, Shuling - HONG, Hanlie - HUANG, Xianyu - FANG, Qian - YIN, Ke - WANG, Chaowen - ZHANG, Yiming - CHENG, Liuling - ALGEO, Thomas J. The role of organo-clay associations in limiting organic matter decay: Insights from the Dajiuhu peat soil, central China. In *GEODERMA*. ISSN 0016-7061, 2018, vol. 320, no., pp. 149-160., Registrované v: WOS
2. [1.1] ZHANG, Lin - CHEN, Jienan - YU, Wenji - ZHAO, Qingfeng - LIU, Jin. Antimicrobial Nanocomposites Prepared from Montmorillonite/Ag+/Quaternary Ammonium Nitrate. In *JOURNAL OF NANOMATERIALS*. ISSN 1687-4110, 2018, vol., no., pp., Registrované v: WOS
- ADCA348 SMRČOK, Ľubomír - TUNEGA, Daniel - RAMIREZ-CUESTA, Anibal Javier - SCHOLTZOVA, Eva. The combined inelastic neutron scattering and solid state DFT study of hydrogen atoms dynamics in a highly ordered kaolinite. In *Physics and Chemistry of Minerals*, 2010, vol. 37, no. 8, p. 571-579. (2009: 1.597 - IF, karentované - CCC). (2010 - Current Contents).
- Citácie:
1. [1.1] DOS SANTOS, E. C. - GATES, W. P. - MICHELS, L. - JURANYI, F. - MIKKELSEN, A. - DA SILVA, G. J. - FOSSUM, J. O. - BORDALLO, H. N. The pH influence on the intercalation of the bioactive agent ciprofloxacin in fluorohectorite. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 166, no., pp. 288-298., Registrované v: WOS
2. [1.1] JIGE, Mayumi - TAKAGI, Tetsuichi - TAKAHASHI, Yoshio - KURISU, Minako - TSUNAZAWA, Yuki - MORIMOTO, Kazuya - HOSHINO, Mihoko - TSUKIMURA, Katsuhiro. Fe-kaolinite in granite saprolite beneath sedimentary kaolin deposits: A mode of Fe substitution for Al in kaolinite. In *AMERICAN MINERALOGIST*. ISSN 0003-004X, 2018, vol. 103, no. 7, pp. 1126-1135., Registrované v: WOS
3. [1.1] TABOROSI, Attila - SZILAGYI, Robert K. - ZSIRKA, Balazs - FONAGY, Orsolya - HORVATH, Erzsebet - KRISTOF, Janos. Molecular Treatment of Nano-Kaolinite Generations. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 12, pp. 7151-7167., Registrované v: WOS
- ADCA349 SMRČOK, Ľubomír - TUNEGA, Daniel - RAMIREZ-CUESTA, Anibal Javier - IVANOV, Alexander - VALÚCHOVÁ, Jana. The combined inelastic neutron scattering (INS) and solid-state DFT study of hydrogen-atoms dynamics in kaolinite-dimethylsulfoxide intercalate. In *Clays and Clay Minerals*, 2010, vol. 58, no. 1, p. 52-61. (2009: 1.431 - IF, karentované - CCC). (2010 - Current Contents). ISSN 0009-8604.
- Citácie:
1. [1.1] MASHEANE, Monaheng - NTHUNYA, Lebea - MUBIAYI, Mukuna - THAMAE, Timothy - MHLANGA, Sabelo. Physico-chemical characteristics of some Lesotho's clays and their assessment for suitability in ceramics production. In *PARTICULATE SCIENCE AND TECHNOLOGY*. ISSN 0272-6351, 2018, vol. 36, no. 1, pp. 117-122., Registrované v: WOS
2. [1.1] TABOROSI, Attila - SZILAGYI, Robert K. - ZSIRKA, Balazs - FONAGY, Orsolya - HORVATH, Erzsebet - KRISTOF, Janos.

Molecular Treatment of Nano-Kaolinite Generations. In INORGANIC CHEMISTRY. ISSN 0020-1669, 2018, vol. 57, no. 12, pp. 7151-7167., Registrované v: WOS

- ADCA350 SMRČOK, Ľubomír - SLÁDKOVIČOVÁ, Mariana - LANGER, Vratislav - WILSON, Chick C. - KOŇŠ, Miroslav. On hydrogen bonding in 1,6-anhydro-beta-D-glucopyranose (levoglucosan): X-ray and neutron diffraction and DFT study. In *Acta Crystallographica Section B*, 2006, vol. 62, p. 912-918. ISSN 0108-7681.

Citácie:

- [1.1] HECZKO, Dawid - KAMINSKA, Ewa - MINECKA, Aldona - DZIENIA, Andrzej - JURKIEWICZ, Karolina - TARNACKA, Magdalena - TALIK, Agnieszka - KAMINSKI, Kamil - PALUCH, Marian. High-pressure dielectric studies on 1,6-anhydro-beta-D-mannopyranose (plastic crystal) and 2,3,4-tri-O-acetyl-1,6-anhydro-beta-D-glucopyranose (canonical glass). In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 20, pp., Registrované v: WOS
- [1.1] JANOSZKA, Katarzyna. Determination of biomass burning tracers in air samples by GC/MS. In *X-TH SCIENTIFIC CONFERENCE AIR PROTECTION IN THEORY AND PRACTICE*. ISSN 2267-1242, 2018, vol. 28, no., pp., Registrované v: WOS
- [1.1] NISHIYAMA, Yoshiharu. Molecular interactions in nanocellulose assembly. In *PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A-MATHEMATICAL PHYSICAL AND ENGINEERING SCIENCES*. ISSN 1364-503X, 2018, vol. 376, no. 2112, pp., Registrované v: WOS
- [1.1] ROTHER, Christina - GUTMANN, Alexander - GUDIMINCHI, Ramakrishna - WEBER, Hansjoerg - LEPAK, Alexander - NIDETZKY, Bernd. Biochemical Characterization and Mechanistic Analysis of the Levoglucosan Kinase from *Lipomyces starkeyi*. In *CHEMBIOCHEM*. ISSN 1439-4227, 2018, vol. 19, no. 6, pp. 596-603., Registrované v: WOS
- [1.1] SUGIURA, Masayuki - NAKAHARA, Moe - YAMADA, Chihaya - ARAKAWA, Takatoshi - KITAOKA, Motomitsu - FUSHINOBU, Shinya. Identification, functional characterization, and crystal structure determination of bacterial levoglucosan dehydrogenase. In *JOURNAL OF BIOLOGICAL CHEMISTRY*, 2018, vol. 293, no. 45, pp. 17375-17386., Registrované v: WOS
- [1.1] URIARTE, Iciar - ECIJA, Patricia - LOZADA-GARCIA, Rolando - CARCABAL, Pierre - COCINERO, Emilio J. Investigating the Conformation of the Bridged Monosaccharide Levoglucosan. In *CHEMPHYSICHEM*. ISSN 1439-4235, 2018, vol. 19, no. 6, pp. 766-773., Registrované v: WOS

- ADCA351 SON, H.L. - SUWANNACHOT, Y. - BUJDÁK, Juraj - RODE, B.M. Salt-induced peptide formation from amino acids in the presence of clays and related catalysts. In *Inorganica Chimica Acta*, 1998, vol. 272, no. 1-2, p. 89-94. (1997: 1.202 - IF, karentované - CCC). (1998 - Current Contents, WOS, SCOPUS). ISSN 0020-1693.

Citácie:

- [1.1] GREGOIRE, Brian - GREENWELL, H. Christopher - FRASER, Donald G. Peptide Formation on Layered Mineral Surfaces: The Key Role of Brucite-like Minerals on the Enhanced Formation of Alanine Dipeptides. In *ACS EARTH AND SPACE CHEMISTRY*. ISSN 2472-3452, 2018, vol. 2, no. 8, pp. 852-862., Registrované v: WOS
- [1.1] KITADAI, Norio - MARUYAMA, Shigenori. Origins of building blocks of life: A review. In *GEOSCIENCE FRONTIERS*. ISSN 1674-9871, 2018, vol. 9, no. 4, pp. 1117-1153., Registrované v: WOS

- ADCA352 SOSA, C. - NOGA, Jozef - BARTLETT, Rodney J. A study of the Be₂ potential curve using the full (CCSDT) coupled-cluster method: The importance of T₄ clusters. In *Journal of Chemical Physics*, 1988, vol. 88, no. 9, p. 5974-5976. ISSN 0021-9606.

Citácie:

- [1.1] LABANC, Daniel - SULKA, Martin - PITONAK, Michal - CERNUSAK, Ivan - URBAN, Miroslav - NEOGRADY, Pavel. Benchmark CCSD(T) and DFT study of binding energies in Be₇-12: in search of reliable DFT functional for beryllium clusters. In *MOLECULAR PHYSICS*. ISSN 0026-8976, 2018, vol. 116, no. 10, pp. 1259-1274., Registrované v: WOS
- [1.1] MAGOULAS, Ilias - BAUMAN, Nicholas P. - SHEN, Jun - PIECUCH, Piotr. Application of the CC(P;Q) Hierarchy of CoupledCluster Methods to the Beryllium Dimer. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 5, pp. 1350-1368., Registrované v: WOS
- [1.1] REINHARDT, Peter - TOULOUSE, Julien - SAVIN, Andreas. Range-separated density-functional theory applied to the beryllium dimer and trimer. In *THEORETICAL CHEMISTRY ACCOUNTS*. ISSN 1432-881X, 2018, vol. 137, no. 12, pp., Registrované v: WOS
- [1.1] URBAN, Miroslav - BLASKO, Martin - CERNUSAK, Ivan - NEOGRADY, Pavel - PITONAK, Michal. Chemical Bond and Intermolecular Interactions. In *CHEMISKE LISTY*. ISSN 0009-2770, 2018, vol. 112, no. 10, pp. 683-692., Registrované v: WOS

- ADCA353 STRAKA, Martin - KORENKO, Michal - LISÝ, František - SZATMÁRY, Lórant. Electrochemistry of samarium in lithium-beryllium fluoride salt mixture. In *Journal of Rare Earths*, 2011, vol. 29, no. 8, p. 798-803. (2010: 1.086 - IF). ISSN 1002-0721.

Citácie:

- [1.1] CHESSER, Ryan - GUO, Shaoqiang - ZHANG, Jinsuo. Electrochemical behavior of dysprosium and lanthanum in molten LiF-NaF-KF (Flink) salt. In *ANNALS OF NUCLEAR ENERGY*. ISSN 0306-4549, 2018, vol. 120, no., pp. 246-252., Registrované v: WOS
- [1.1] GUO, Shaoqiang - ZHANG, Jinsuo - WU, Wei - ZHOU, Wentao. Corrosion in the molten fluoride and chloride salts and materials development for nuclear applications. In *PROGRESS IN MATERIALS SCIENCE*. ISSN 0079-6425, 2018, vol. 97, no., pp. 448-487., Registrované v: WOS
- [1.1] YAN, Qi-Cao - GUO, Xing-Min. Preparation and characterization of Sm₂Fe₁₇ alloy in LiF-CaF₂-SmF₃ molten salt. In *JOURNAL OF ALLOYS AND COMPOUNDS*. ISSN 0925-8388, 2018, vol. 747, no., pp. 994-1001., Registrované v: WOS

- ADCA354 SVOBODA, Roman - MÁLEK, Jiří - LIŠKA, Marek. Correlation between the structure and relaxation dynamics of (GeS₂)_y(Sb₂S₃)_{1-y} glassy matrices. In *Journal of Non-Crystalline Solids*, 2018, vol. 479, p. 113-119. (2017: 2.488 - IF, Q1 - JCR, 0.722 - SJR, Q1 - SJR, karentované - CCC). (2018 - Current Contents). ISSN 0022-3093.

Citácie:

1. [1.1] FRAENKL, Max - FRUMAROVA, Bozena - PODZEMNA, Veronika - SLANG, Stanislav - BENES, Ludvik - VLCEK, Milan - WAGNER, Tomas. How silver influences the structure and physical properties of chalcogenide glass (GeS₂)(50)(Sb₂S₃)(50). In *JOURNAL OF NON-CRYSTALLINE SOLIDS*. ISSN 0022-3093, 2018, vol. 499, no., pp. 412-419., Registrované v: WOS
- ADCA355 SZATMÁRY, Lóránt - BAKARDJIEVA, Snežana - ŠUBRT, Jan - BEZDIČKA, P. - JIRKOVSKÝ, Jaromír - BASTL, Zdeněk - BREZOVÁ, Vlasta - KORENKO, Michal. Sulphur doped nanoparticles of TiO₂. In *Catalysis Today*, 2011, vol. 161, no. 1, p. 23-28. (2010: 2.993 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0920-5861.
- Citácie:
1. [1.1] NASIRIAN, M. - LIN, Y. P. - BUSTILLO-LECOMPTE, C. F. - MEHRVAR, M. Enhancement of photocatalytic activity of titanium dioxide using non-metal doping methods under visible light: a review. In *INTERNATIONAL JOURNAL OF ENVIRONMENTAL SCIENCE AND TECHNOLOGY*. ISSN 1735-1472, 2018, vol. 15, no. 9, pp. 2009-2032., Registrované v: WOS
2. [1.1] POPA, Adriana - STEFAN, Maria - TOLOMAN, Dana - PANA, Ovidiu - MESAROS, Amalia - LEOSTEAN, Cristian - MACAVEI, Sergiu - MARINCAS, Olivian - SUCIU, Ramona - BARBU-TUDORAN, Lucian. Fe₃O₄-TiO₂: Gd nanoparticles with enhanced photocatalytic activity and magnetic recyclability. In *POWDER TECHNOLOGY*. ISSN 0032-5910, 2018, vol. 325, no., pp. 441-451., Registrované v: WOS
3. [1.1] XIANG, Liyun - YA, Jing - LI, Lixia - LIU, Zhifeng. Effect on the Photocatalytic Activity of TiO₂NTs Under Visible Light of Synergistic Effect of Ti³⁺ and S. In *NANO*. ISSN 1793-2920, 2018, vol. 13, no. 2, pp., Registrované v: WOS
- ADCA356 ŠAJGALÍK, Pavol - HNATKO, Miroslav - ČOPAN, Peter - LENČEŠ, Zoltán - HUANG, J.-L. Influence of graphite additives on wear properties of hot pressed Si₃N₄ ceramics. In *Journal of the Ceramic Society of Japan*, 2006, vol. 114, no. 1335, p. 1061-1068.
- Citácie:
1. [1.1] HAN, Yao - LI, Shuang - ZHU, Tianbin - WU, Weiwei - AN, Di - HU, Feng - ZHAI, Fengrui - XIE, Zhipeng. Enhanced toughness and reliability of Si₃N₄-SiCw composites under oscillatory pressure sintering. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 11, pp. 12169-12173., Registrované v: WOS
- ADCA357 ŠAJGALÍK, Pavol - SEDLÁČEK, Jaroslav - LENČEŠ, Zoltán - DUSZA, Ján - LIN, Hua-Tay. Additive-free hot-pressed silicon carbide ceramics - A material with exceptional mechanical properties. In *Journal of the European Ceramic Society*, 2016, vol. 36, no. 6, p. 1333-1341. (2015: 2.933 - IF, Q1 - JCR, 1.150 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0955-2219.
- Citácie:
1. [1.1] DU PREEZ, S. P. - BEUKES, J. P. - VAN ZYL, P. G. - TANGSTAD, M. - TIEDT, L. R. Silicon Carbide Formation Enhanced by In-Situ-Formed Silicon Nitride: An Approach to Capture Thermal Energy of CO-Rich Off-Gas Combustion. In *METALLURGICAL AND MATERIALS TRANSACTIONS B-PROCESS METALLURGY AND MATERIALS PROCESSING SCIENCE*. ISSN 1073-5615, 2018, vol. 49, no. 6, pp. 3151-3163., Registrované v: WOS
2. [1.1] SEO, Yu-Kwang - EOM, Jung-Hye - KIM, Young-Wook. Process-tolerant pressureless-sintered silicon carbide ceramics with alumina-yttria-calcia-strontia. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 2, pp. 445-452., Registrované v: WOS
3. [1.1] YASAR, Zeynep Aygüzer - DELUCCA, Vincent A. - HABER, Richard A. Influence of oxygen content on the microstructure and mechanical properties of SPS SiC. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 18, pp. 23248-23253., Registrované v: WOS
- ADCA358 ŠAJGALÍK, Pavol - DUSZA, Ján - HOFFMANN, M.J. Relationship between microstructure toughening mechanisms and fracture toughness of reinforced Si₃N₄ ceramics. In *Journal of the American Ceramic Society*, 1995, vol. 78, no. 10, p. 2619-2624. ISSN 0002-7820.
- Citácie:
1. [1.1] GUO, Wei - XU, Xiaomin - YAN, Chen - JIANG, Cuifeng - JIANG, Jinhai - LIU, Tiantian. INFLUENCE OF Al₂O₃ ON PREPARING POROUS SILICON NITRIDE BASED CERAMIC FROM RICE HUSK. In *FRESENIUS ENVIRONMENTAL BULLETIN*. ISSN 1018-4619, 2018, vol. 27, no. 8, pp. 5647-5654., Registrované v: WOS
2. [1.1] HAN, Yao - LI, Shuang - ZHU, Tianbin - WU, Weiwei - AN, Di - HU, Feng - ZHAI, Fengrui - XIE, Zhipeng. Enhanced toughness and reliability of Si₃N₄-SiCw composites under oscillatory pressure sintering. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 11, pp. 12169-12173., Registrované v: WOS
3. [1.1] HAN, Yao - XIE, Zhipeng - LI, Shuang - ZHU, Tianbin - WU, Weiwei - AN, Di - HU, Feng - ZHAI, Fengrui. Optimum sintering temperature of high quality silicon nitride ceramics under oscillatory pressure. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 6, pp. 6949-6952., Registrované v: WOS
4. [1.1] RAHAMAN, Mohamed - XIAO, Wei. Silicon nitride bioceramics in healthcare. In *INTERNATIONAL JOURNAL OF APPLIED CERAMIC TECHNOLOGY*. ISSN 1546-542X, 2018, vol. 15, no. 4, pp. 861-872., Registrované v: WOS
5. [1.1] STROBL, Stefan - ADLMANN, Franz-Alois - SUPANCIC, Peter - LUBE, Tanja - DANZER, Robert - SCHOEPL, Oskar. Fracture toughness of silicon nitride balls via thermal shock. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 4, pp. 1278-1287., Registrované v: WOS
6. [1.1] WANG, Xuechun - SONG, Renfeng - CHEN, Yinjie - ZHAO, Yunhui - ZHU, Kongying - YUAN, Xiaoyan. Mechanical properties of polypropylene by diversely compatibilizing with titanate whiskers in composites. In *COMPOSITES SCIENCE AND TECHNOLOGY*. ISSN 0266-3538, 2018, vol. 164, no., pp. 103-109., Registrované v: WOS
- ADCA359 ŠIMEG VETERNÍKOVÁ, Jana - DEGMOVÁ, J. - PEKARČÍKOVÁ, M. - ŠIMKO, František - PETRISKA, Martin - SKARBA, M. - MIKULA, P. - PUPALA, Martin. Thermal stability study for candidate stainless steels of GEN IV reactors. In *Applied Surface Science*, 2016, vol. 387, p. 965-970. (2015: 3.150 - IF, Q1 - JCR, 0.914 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0169-4332.
- Citácie:
1. [1.1] TUNC, Guven - SAHIN, Hacı Mehmet - SAHIN, Sumer. Evaluation of the radiation damage parameters of ODS steel alloys

in the first wall of deuterium-tritium fusion-fission (hybrid) reactors. In *INTERNATIONAL JOURNAL OF ENERGY RESEARCH*. ISSN 0363-907X, 2018, vol. 42, no. 1, pp. 198-206., Registrované v: WOS

2. [1.1] XU, Chi - CHEN, Wei-Ying - CHEN, Yiren - YANG, Yong. Microstructural evolution of NF709 austenitic stainless steel under in-situ ion irradiations at room temperature, 300, 400, 500 and 600 degrees C. In *JOURNAL OF NUCLEAR MATERIALS*. ISSN 0022-3115, 2018, vol. 509, no., pp. 644-653., Registrované v: WOS

3. [1.1] ZHAO, Dandan - LI, Shilei - WANG, Yanli - LIU, Fang - WANG, Xitao. Investigation of ion irradiation hardening behaviors of tempered and long-term thermal aged T92 steel. In *JOURNAL OF NUCLEAR MATERIALS*. ISSN 0022-3115, 2018, vol. 511, no., pp. 191-199., Registrované v: WOS

ADCA360 ŠIMKO, František - MACKOVÁ, Iveta - NETRIOVÁ, Zuzana. Density of the systems (NaF / AlF₃)–AlPO₄ and (NaF / AlF₃)–NaVO₃. In *Chemical papers*, 2011, vol. 65, no. 1, p. 85-89. (2010: 0.754 - IF, karentované - CCC). (2011 - Current Contents). ISSN 0366-6352.

Citácie:

1. [1.1] KUBIKOVA, Blanka - MLYNARIKOVA, Jarmila - BENES, Ondrej - MIKSIKOVA, Eva - PRISCAK, Jozef - TOSOLIN, Alberto - BOCA, Miroslav. Physico-chemical properties of the system (LiF-NaF)(eut)-LaF₃ Phase equilibria, density and volume properties, electrical conductivity and surface tension. In *JOURNAL OF MOLECULAR LIQUIDS*. ISSN 0167-7322, 2018, vol. 268, no., pp. 754-761., Registrované v: WOS

ADCA361 ŠUCHA, Vladimír - CZÍMEROVÁ, Adriana - BUJDÁK, Juraj. Surface properties of illite-smectite minerals as detected by interactions with rhodamine 6G dye. In *Clays and Clay Minerals*, 2009, vol. 57, no. 3, p. 361-370. (2008: 1.171 - IF). ISSN 0009-8604.

Citácie:

1. [1.1] KULIGIEWICZ, Artur - DERKOWSKI, Arkadiusz - SRODON, Jan - GIONIS, Vassilis - CHRYSSIKOS, Georgios D. The charge of wettable illite-smectite surfaces measured with the O-D method. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 161, no., pp. 354-363., Registrované v: WOS

ADCA362 ŠUCHA, Vladimír - KRAUS, Ivan - MADEJOVÁ, Jana. Ammonium illite from anchimetamorphic shales associated with anthracite in the zemplinicum of the Western Carpathians. In *Clay Minerals*, 1994, vol. 29, no. 3, p. 369-377. ISSN 0009-8558.

Citácie:

1. [1.1] ANDRADE, Gabriel R. P. - CUADROS, Javier - PARTITI, Carmen S. M. - COHEN, Renato - VIDAL-TORRADO, Pablo. Sequential mineral transformation from kaolinite to Fe-illite in two Brazilian mangrove soils. In *GEODERMA*. ISSN 0016-7061, 2018, vol. 309, no., pp. 84-99., Registrované v: WOS

2. [1.1] BAULUZ, Blanca - NIETO, Fernando. Ammonium-bearing micas in very low-grade metapelites: micro- and nano-texture and composition. In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 2, pp. 105-116., Registrované v: WOS

3. [1.1] DAI, Shifeng - JI, Dongping - WARD, Cohn R. - FRENCH, David - HOWER, James C. - YAN, Xiaoyun - WEI, Qiang. Mississippian anthracites in Guangxi Province, southern China: Petrological, mineralogical, and rare earth element evidence for high-temperature solutions. In *INTERNATIONAL JOURNAL OF COAL GEOLOGY*. ISSN 0166-5162, 2018, vol. 197, no., pp. 84-114., Registrované v: WOS

ADCA363 ŠUCHA, Vladimír - ELSASS, Francoise - EBERL, Dennis D. - KUCHTA, L. - MADEJOVÁ, Jana - GATES, W.P. - KOMADEL, Peter. Hydrothermal synthesis of ammonium illite. In *American Mineralogist*, 1998, vol. 83, no. 1-2, p. 58-67. ISSN 0003-004X.

Citácie:

1. [1.1] CUADROS, Javier - CESARANO, Mara - DUBBIN, William - SMITH, Stuart W. - DAVEY, Alexandra - SPIRO, Baruch - BURTON, Rodney G. O. - JUNGBLUT, Anne D. Slow weathering of a sandstone-derived Podzol (Falkland Islands) resulting in high content of a non-crystalline silicate. In *AMERICAN MINERALOGIST*. ISSN 0003-004X, 2018, vol. 103, no. 1, pp. 109-124., Registrované v: WOS

2. [1.1] EHLMANN, Bethany L. - HODYSS, Robert - BRISTOW, Thomas F. - ROSSMAN, George R. - AMMANNITO, Eleonora - DE SANCTIS, M. Cristina - RAYMOND, Carol A. Ambient and cold-temperature infrared spectra and XRD patterns of ammoniated phyllosilicates and carbonaceous chondrite meteorites relevant to Ceres and other solar system bodies. In *METEORITICS & PLANETARY SCIENCE*. ISSN 1086-9379, 2018, vol. 53, no. 9, pp. 1884-1901., Registrované v: WOS

3. [1.1] JO, Jaeguk - YAMANAKA, Toshiro - KASHIMURA, Tomoki - OKUNISHI, Yusuke - KUWAHARA, Yoshihiro - KADOTA, Isao - MIYOSHI, Youko - ISHIBASHI, Jun-Ichiro - CHIBA, Hitoshi. Mineral nitrogen isotope signature in clay minerals formed under high ammonium environment conditions in sediment associated with ammonium-rich sediment-hosted hydrothermal system. In *GEOCHEMICAL JOURNAL*. ISSN 0016-7002, 2018, vol. 52, no. 4, pp. 317-333., Registrované v: WOS

4. [1.1] SIDORENKO, A. Yu. - KRAVTSOVA, A. V. - AHO, A. - HEINMAA, I. - KUZNETSOVA, T. F. - MURZIN, D. Yu. - AGABEKOV, V. E. Catalytic isomerization of alpha-pinene oxide in the presence of acid-modified clays. In *MOLECULAR CATALYSIS*. ISSN 2468-8231, 2018, vol. 448, no., pp. 18-29., Registrované v: WOS

5. [1.1] SIDORENKO, A. Yu. - KRAVTSOVA, A. V. - WARNA, J. - AHO, A. - HEINMAA, I. - IL'INA, I. V. - ARDASHOV, O. V. - VOLCHO, K. P. - SALAKHUTDINOV, N. F. - MURZIN, D. Yu. - AGABEKOV, V. E. Preparation of octahydro-2H-chromen-4-ol with analgesic activity from isopulegol and thiophene-2-carbaldehyde in the presence of acid-modified clays. In *MOLECULAR CATALYSIS*. ISSN 2468-8231, 2018, vol. 453, no., pp. 139-148., Registrované v: WOS

ADCA364 ŠUCHA, Vladimír - UHLÍK, Peter - MADEJOVÁ, Jana - PETIT, Sabine - KRAUS, Ivan - PUŠKELOVÁ, Ľubica. Particle properties of hydrothermal ammonium-bearing illite-smectite. In *Clays and Clay Minerals*, 2007, vol. 55, no. 1, p. 36-44. (2006: 1.423 - IF). ISSN 0009-8604.

Citácie:

1. [1.1] JO, Jaeguk - YAMANAKA, Toshiro - KASHIMURA, Tomoki - OKUNISHI, Yusuke - KUWAHARA, Yoshihiro - KADOTA, Isao - MIYOSHI, Youko - ISHIBASHI, Jun-Ichiro - CHIBA, Hitoshi. Mineral nitrogen isotope signature in clay minerals formed under high ammonium environment conditions in sediment associated with ammonium-rich sediment-hosted hydrothermal system. In *GEOCHEMICAL JOURNAL*. ISSN 0016-7002, 2018, vol. 52, no. 4, pp. 317-333., Registrované v: WOS

2. [1.1] KRISSANSEN-TOTTON, Joshua - OLSON, Stephanie - CATLING, David C. Disequilibrium biosignatures over Earth

history and implications for detecting exoplanet life. In SCIENCE ADVANCES. ISSN 2375-2548, 2018, vol. 4, no. 1, pp., Registrované v: WOS

- ADCA365 ŠUCHA, Vladimír - ŠRODOŇ, J. - CLAUER, N. - ELSASS, Françoise - EBERL, Dennis D. - KRAUS, Ivan - MADEJOVÁ, Jana. Weathering of smectite and illite-smectite under temperate climatic conditions. In Clay Minerals, 2001, vol. 36, no. 3, p. 403-419. (2001 - Current Contents). ISSN 0009-8558.

Citácie:

1. [1.1] VLCEK, Vitezslav - POSPISILOVA, Lubica - UHLIK, Peter. Mineralogy and Chemical Composition of Cryosols and Andosols in Antarctica. In SOIL AND WATER RESEARCH. ISSN 1801-5395, 2018, vol. 13, no. 2, pp. 61-73., Registrované v: WOS

- ADCA366 ŠVANČÁREK, Peter - KLEMENT, Róbert - GALUSEK, Dušan. Photoluminescence of (ZnO)X-Z(SiO₂)Y:(MnO)Z green phosphors prepared by direct thermal synthesis: The effect of ZnO/SiO₂ ratio and Mn²⁺ concentration of luminescence. In Ceramics International, 2016, vol. 42, no. 15, p. 16852-16860. (2015: 2.758 - IF, Q1 - JCR, 0.846 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 0272-8842.

Citácie:

1. [1.1] YU, Panlong - TIAN, Lianhua. A single-composition tunable-emission phosphor NaTaOGeO₄:Mn²⁺,Pr³⁺. In OPTICAL MATERIALS. ISSN 0925-3467, 2018, vol. 85, no., pp. 444-450., Registrované v: WOS

- ADCA367 ŠVANČÁREK, Peter - GALUSEK, Dušan - CALVERT, Clair - LOUGHRAN, Fiona - BROWN, Andy - BRYDSON, R. - RILEY, F.L. A comparison of the microstructure and mechanical properties of two liquid phase sintered aluminas containing different molar ratios of calcia-silica sintering additives. In Journal of the European Ceramic Society, 2004, vol. 24, no. 12, p. 3453-3463. ISSN 0955-2219.

Citácie:

1. [1.1] GOPINATH, K. G. S. - PAL, Soumen - TAMBE, Pankaj. Prediction of Hardness and Fracture Toughness in Liquid-Phase Sintered Alumina System Using Gaussian Process Regression and Minimax Probability Machine Regression. In MATERIALS TODAY-PROCEEDINGS. ISSN 2214-7853, 2018, vol. 5, no. 5, pp. 12223-12232., Registrované v: WOS

2. [1.1] YOU, Jiali - YANG, Tao - FENG, Dandan - LI, Zhihong. Synthesis and two-step sintering behavior of solution derived corundum abrasives with plate-like grains. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 11, pp. 12615-12620., Registrované v: WOS

- ADCA368 ŠVANČÁREK, Peter - SCHWENDT, Peter - TATIERSKY, Jozef - KUTÁ SMATANOVÁ, Ivana - MAREK, Jaromír. Oxo peroxo glycolato complexes of vanadium(V). Crystal structure of (NBu₄)(2)[V₂O₂(O-2)(2)(C₂H₂O₃)(2)]center dot H₂O. In Monatshefte für Chemie, 2000, vol. 131, no. 2, p. 145-154. ISSN 0026-9247.

Citácie:

1. [1.1] MCLAUCHLAN, Craig C. - MURAKAMI, Heide A. - WALLACE, Craig A. - CRANS, Debbie C. Coordination environment changes of the vanadium in vanadium-dependent haloperoxidase enzymes. In JOURNAL OF INORGANIC BIOCHEMISTRY. ISSN 0162-0134, 2018, vol. 186, no., pp. 267-279., Registrované v: WOS

- ADCA369 TAIFAN, William E. - BUČKO, Tomáš - BALTRUSAITIS, Jonas. Catalytic conversion of ethanol to 1,3-butadiene on MgO: A comprehensive mechanism elucidation using DFT calculations. In Journal of Catalysis, 2017, vol. 346, p. 78-91. (2016: 6.844 - IF, Q1 - JCR, 2.451 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0021-9517.

Citácie:

1. [1.1] BING, Weihang - ZHENG, Lei - HE, Shan - RAO, Deming - XU, Ming - ZHENG, Lirong - WANG, Bin - WANG, Yangdong - WEI, Min. Insights on Active Sites of CaAl-Hydrotalcite as a High-Performance Solid Base Catalyst toward Aldol Condensation. In ACS CATALYSIS. ISSN 2155-5435, 2018, vol. 8, no. 1, pp. 656-664., Registrované v: WOS

2. [1.1] FARRAR-TOBAR, Ronald A. - WEI, Zhihong - JIAO, Haijun - HINZE, Sandra - DE VRIES, Johannes G. Selective Base-free Transfer Hydrogenation of α -Unsaturated Carbonyl Compounds using iPrOH or EtOH as Hydrogen Source. In CHEMISTRY-A EUROPEAN JOURNAL. ISSN 0947-6539, 2018, vol. 24, no. 11, pp. 2725-2734., Registrované v: WOS

3. [1.1] WANG, Fangfang - XIA, Wei - MU, Xichuan - CHEN, Kun - SI, Huimin - LI, Zhihao. A combined experimental and theoretical study on ethanol conversion to propylene over Y/ZrO₂ catalyst. In APPLIED SURFACE SCIENCE. ISSN 0169-4332, 2018, vol. 439, no., pp. 405-412., Registrované v: WOS

4. [1.1] XIA, Wei - WANG, Fangfang - WANG, Longxiang - WANG, Junguo - MU, Xichuan - CHEN, Kun. High Performance SiO₂-ZrO₂ Binary Oxide for Ethanol Conversion to Ethylene. In CATALYSIS LETTERS. ISSN 1011-372X, 2018, vol. 148, no. 10, pp. 3024-3034., Registrované v: WOS

5. [1.1] ZHANG, Minhua - ZHUANG, Jianyu - YU, Yingzhe. A DFT study on ZrO₂ surface in the process of ethanol to 1,3-butadiene: A comprehensive mechanism elucidation. In APPLIED SURFACE SCIENCE. ISSN 0169-4332, 2018, vol. 458, no., pp. 1026-1034., Registrované v: WOS

- ADCA370 TATARKO, Peter - KAŠIAROVÁ, Monika - DUSZA, Ján - MORGIEL, Jerzy - ŠAJGALÍK, Pavol - HVIZDOŠ, Pavol. Wear resistance of hot-pressed Si₃N₄/SiC micro/nanocomposites sintered with rare-earth oxide additives. In Wear : an international journal on the science and technology of friction, lubrication and wear, 2010, vol. 269, p. 867-874. (2009: 1.771 - IF, karentované - CCC). (2010 - Current Contents). ISSN 0043-1648.

Citácie:

1. [1.1] LI, Zhenbao - CAO, Yejie - HE, Jiabei - WANG, Yiguang. Mechanical and tribological performances of C-SiC nanocomposites synthesized from polymer-derived ceramics sintered by spark plasma sintering. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 12, pp. 14335-14341., Registrované v: WOS

2. [1.1] YE, Chaochao - YUE, Xinyan - JIANG, Yan - LI, Hongjun - RU, Hongqiang. Effect of different preparation methods on the

microstructure and mechanical properties of Si₃N₄ ceramic composites. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 4, pp. 3664-3671., Registrované v: WOS

- ADCA371 TATARKO, Peter - KAŠIAROVÁ, Monika - CHLUP, Zdeněk - DUSZA, Ján - ŠAJGALÍK, Pavol - VÁVRA, Ivo. Influence of rare-earth oxide additives and SiC nanoparticles on the wear behaviour of Si₃N₄-based composites at temperatures up to 900 C. In *Wear : an international journal on the science and technology of friction, lubrication and wear*, 2013, vol. 300, p. 155-162. (2012: 1.262 - IF, 1.360 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 0043-1648.

Citácie:

1. [1.1] LIU, Jiongjie - YANG, Jun - YU, Yuan - SUN, Qichun - QIAO, Zhuhui - LIU, Weimin. Self-Lubricating Si₃N₄-based composites toughened by in situ formation of silver. In *CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 12, pp. 14327-14334., Registrované v: WOS*
2. [1.1] WANG, Junhai - LI, Ting - YAN, Tingting - ZHANG, Lixiu - ZHANG, Ke - QU, Xin. Role of Magnesium Perrhenate in an Oil/Solid Mixed System for Tribological Application at Various Temperatures. In *MATERIALS. ISSN 1996-1944, 2018, vol. 11, no. 9, pp., Registrované v: WOS*
3. [1.1] WANG, Junhai - LU, Bing - ZHANG, Lixiu - LI, Ting - YAN, Tingting - LI, Mengxu. An investigation on the tribological properties of Co(ReO₄)(2)/MoS₂ composite as potential lubricating additive at various temperatures. In *MATERIALS RESEARCH EXPRESS. ISSN 2053-1591, 2018, vol. 5, no. 2, pp., Registrované v: WOS*

- ADCA372 TATARKO, Peter - KAŠIAROVÁ, Monika - DUSZA, Ján - ŠAJGALÍK, Pavol. Influence of rare-earth oxide additives on the oxidation resistance of Si₃N₄-SiC nanocomposites. In *Journal of the European Ceramic Society*, 2013, vol. 33, p. 2259-2268. (2012: 2.360 - IF, 1.305 - SJR, karentované - CCC). (2013 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] XU, Weiwei - YUAN, Juntang - YIN, Zengbin - CHEN, Mingdan - WANG, Zhenhua. Effect of metal phases on microstructure and mechanical properties of Si₃N₄-based ceramic tool materials by microwave sintering. In *CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 16, pp. 19872-19878., Registrované v: WOS*

- ADCA373 TATARKO, Peter - LOJANOVÁ, Š. - DUSZA, Ján - ŠAJGALÍK, Pavol. Influence of various rare-earth oxide additives on microstructure and mechanical properties of silicon nitride based nanocomposites. In *Materials Science and Engineering A - Structural Materials Properties Microstructure and Processing*, 2010, vol. 527, p. 4771-4778. (2009: 1.901 - IF, karentované - CCC). (2010 - Current Contents). ISSN 0921-5093.

Citácie:

1. [1.1] CAO, Liyan - WANG, Zhenhua - YIN, Zengbin - LIU, Kui - YUAN, Juntang. Investigation on mechanical properties and microstructure of silicon nitride ceramics fabricated by spark plasma sintering. In *MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING. ISSN 0921-5093, 2018, vol. 731, no., pp. 595-602., Registrované v: WOS*
2. [1.1] GUEDES-SILVA, Cecilia Chaves - DORION RODAS, Andrea Cecilia - SILVA, Antonio Carlos - RIBEIRO, Christiane - DE SOUZA CARVALHO, Flavio Machado - HIGA, Olga Zazuco - FERREIRA, Thiago dos Santos. Microstructure, Mechanical Properties and in vitro Biological Behavior of Silicon Nitride Ceramics. In *MATERIALS RESEARCH-IBERO-AMERICAN JOURNAL OF MATERIALS. ISSN 1516-1439, 2018, vol. 21, no. 6, pp., Registrované v: WOS*
3. [1.1] KHODAEI, Mandi - YAGHOBIZADEH, Omid - EHSANI, Naser - BAHARVANDI, Hamid Reza - DASHTI, Alireza. The effect of TiO₂ additive on sinterability and properties of SiC-Al₂O₃-Y₂O₃ composite system. In *CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 14, pp. 16535-16542., Registrované v: WOS*

- ADCA374 TATARKO, Peter - GRASSO, Salvatore - SAUNDERS, Theo G. - FERRARIS, Monica - REECE, Michael J. Flash joining of CVD-SiC coated Cf/SiC composites with a Ti interlayer. In *Journal of the European Ceramic Society*, 2017, vol. 37, no. 13, p. 3841-3848. (2016: 3.454 - IF, Q1 - JCR, 1.142 - SJR, Q1 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0955-2219.

Citácie:

1. [1.1] FITRIANI, Pipit - YOON, Dang-Hyok. Joining of SiCf/SiC using a Ti₃AlC₂ filler and subsequent elimination of the joining layer. In *CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 18, pp. 22943-22949., Registrované v: WOS*
2. [1.1] LOGESH, G. - RASHAD, Mohammed - LODHE, Mangesh - SABU, Ummen - JOSEPH, Andrews - RAJU, K. C. James - BALASUBRAMANIAN, M. Mechanical and dielectric properties of carbon fiber reinforced reaction bonded silicon nitride composites. In *JOURNAL OF ALLOYS AND COMPOUNDS. ISSN 0925-8388, 2018, vol. 767, no., pp. 1083-1093., Registrované v: WOS*
3. [1.1] ZHUANG, Lei - FU, Qian-Gang - YU, Xin. Improved thermal shock resistance of SiCnw/PyC core-shell structure toughened CVD-SiC coating. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY. ISSN 0955-2219, 2018, vol. 38, no. 7, pp. 2808-2814., Registrované v: WOS*

- ADCA375 TUNEGA, Daniel - BUČKO, Tomáš - ZAOUI, Ali. Assessment of ten DFT methods in predicting structures of sheet silicates: Importance of dispersion corrections. In *Journal of Chemical Physics*, 2012, vol. 137, no. 11, p. 114105-1-114105-9. (2011: 3.333 - IF, 1.805 - SJR, karentované - CCC). (2012 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] AKIYAMA, Sohta - MIYAJI, Akimitsu - HAYASHI, Yoshihiro - HIZA, Misao - SEKIGUCHI, Yasumasa - KOYAMA, To-ru - SHIGA, Akinobu - BABA, Toshihide. Selective conversion of ethanol to 1,3-butadiene using germanium talc as catalyst. In *JOURNAL OF CATALYSIS. ISSN 0021-9517, 2018, vol. 359, no., pp. 184-197., Registrované v: WOS*
2. [1.1] CHURAKOV, Sergey V. - LIU, Xiandong. Quantum-chemical modelling of clay mineral surfaces and clay mineral-surface-adsorbate interactions. In *SURFACE AND INTERFACE CHEMISTRY OF CLAY MINERALS, VOL 9. ISSN 1572-4352, 2018, vol. 9, no., pp. 49-87., Registrované v: WOS*

3. [1.1] COLMENERO, Francisco - TIMON, Vicente - BONALES, Laura J. - COBOS, Joaquin. Structural, mechanical and Raman spectroscopic characterization of the layered uranyl silicate mineral, uranophane- α , by density functional theory methods. In *CLAY MINERALS*. ISSN 0009-8558, 2018, vol. 53, no. 3, pp. 377-392., Registrované v: WOS
 4. [1.1] TABOROSI, Attila - SZILAGYI, Robert K. - ZSIRKA, Balazs - FONAGY, Orsolya - HORVATH, Erzsebet - KRISTOF, Janos. Molecular Treatment of Nano-Kaolinite Generations. In *INORGANIC CHEMISTRY*. ISSN 0020-1669, 2018, vol. 57, no. 12, pp. 7151-7167., Registrované v: WOS
 5. [1.1] YAGHOUBI, Alireza - MASENELLI-VARLOT, Karine - BOISRON, Olivier - RAMESH, S. - MELINON, Patrice. Is Graphitic Silicon Carbide (Silagraphene) Stable? In *CHEMISTRY OF MATERIALS*. ISSN 0897-4756, 2018, vol. 30, no. 20, pp. 7234-7244., Registrované v: WOS
 6. [1.1] YANG, Zongyi - LIU, Wenli - ZHANG, He - JIANG, Xinli - MIN, Fanfei. DFT study of the adsorption of 3-chloro-2-hydroxypropyl trimethylammonium chloride on montmorillonite surfaces in solution. In *APPLIED SURFACE SCIENCE*. ISSN 0169-4332, 2018, vol. 436, no., pp. 58-65., Registrované v: WOS
- ADCA376 UHRINOVÁ, Anna - KUCHÁR, Juraj - ORENDÁČOVÁ, Alžbeta - PITOŇÁK, Michal - FEDERIČ, Pavol - NOGA, Jozef - ČERNÁK, Juraj. [Ni(bpy)(mal)(H₂O)₃].H₂O and [Ni(4,4'-dmbpy)(mal)(H₂O)₃].1.5H₂O: syntheses, crystal structures, magnetic properties, and computational study of stacking interactions. In *Journal of coordination chemistry*, 2017, vol. 70, no. 17, p. 2999-3018. (2016: 1.795 - IF, Q3 - JCR, 0.364 - SJR, Q2 - SJR, karentované - CCC). (2017 - Current Contents). ISSN 0095-8972.
- Citácie:
1. [1.1] CERNAK, Juraj - KOCANOVA, Ivana - KUCHAR, Juraj - HILLARD, Elizabeth A. - CLERAC, Rodolphe. Formation of the unprecedented trinuclear [NiCu₂(CN)(8)](4-) complex anion within the crystal structure of [Ni(5,5'-dmbpy)(3)](2)[NiCu₂(CN)(8)]center dot 6H(2)O. In *INORGANIC CHEMISTRY COMMUNICATIONS*. ISSN 1387-7003, 2018, vol. 91, no., pp. 16-19., Registrované v: WOS
- ADCA377 URBAN, Miroslav - NOGA, Jozef - COLE, S.J. - BARTLETT, Rodney J. Towards a full CCSDT model for electron correlation. In *Journal of Chemical Physics*, 1985, vol. 83, no. 8, p. 4041-4046. ISSN 0021-9606.
- Citácie:
1. [1.1] CROCE, Adela E. - COBOS, Carlos J. Quantum-chemical and kinetic study of the reactions of the ClSO₂ radical with H, O, Cl, S, SCl and ClSO₂ in the atmosphere of Venus. In *COMPUTATIONAL AND THEORETICAL CHEMISTRY*. ISSN 2210-271X, 2018, vol. 1140, no., pp. 14-23., Registrované v: WOS
 2. [1.1] DHIFLAOUI, J. - BEJAOUI, M. - FARJALLAH, M. - BERRICHE, H. Investigation of the electronic structure of Be₂+He and Be+He, and static dipole polarisabilities of the helium atom. In *MOLECULAR PHYSICS*. ISSN 0026-8976, 2018, vol. 116, no. 10, pp. 1347-1357., Registrované v: WOS
 3. [1.1] GUO, Yang - RIPLINGER, Christoph - BECKER, Ute - LIAKOS, Dimitrios G. - MINENKOV, Yury - CAVALLO, Luigi - NEESE, Frank. Communication: An improved linear scaling perturbative triples correction for the domain based local pair-natural orbital based singles and doubles coupled cluster method [DLPNO-CCSD(T)]. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 1, pp., Registrované v: WOS
 4. [1.1] HAO, Yongliang - ILIAS, Miroslav - ELIAV, Ephraim - SCHWERTFEGGER, Peter - FLAMBAUM, Victor V. - BORSCHEVSKY, Anastasia. Nuclear anapole moment interaction in BaF from relativistic coupled-cluster theory. In *PHYSICAL REVIEW A*. ISSN 2469-9926, 2018, vol. 98, no. 3, pp., Registrované v: WOS
 5. [1.1] KAPLAN, Ilya G. - MIRANDA, Ulises - TRAKHTENBERG, Leonid I. Study of the In₂O₃ molecule in the free state and in the crystal. In *MOLECULAR PHYSICS*. ISSN 0026-8976, 2018, vol. 116, no. 5-6, pp. 678-685., Registrované v: WOS
 6. [1.1] KOWALSKI, Karol - BRABEC, Jiri - PENG, Bo. Regularized and Renormalized Many-Body Techniques for Describing Correlated Molecular Systems: A Coupled-Cluster Perspective. In *ANNUAL REPORTS IN COMPUTATIONAL CHEMISTRY*, VOL 14. ISSN 1574-1400, 2018, vol. 14, no., pp. 3-45., Registrované v: WOS
 7. [1.1] LISCHKA, Hans - NACHTIGALLOVA, Dana - AQUINO, Adelia J. A. - SZALAY, Peter G. - PLASSER, Felix - MACHADO, Francisco B. C. - BARBATTI, Mario. Multireference Approaches for Excited States of Molecules. In *CHEMICAL REVIEWS*. ISSN 0009-2665, 2018, vol. 118, no. 15, pp. 7293-7361., Registrované v: WOS
 8. [1.1] LYAKH, Dmitry I. Efficient electronic structure theory via hierarchical scale-adaptive coupled-cluster formalism: I. Theory and computational complexity analysis. In *MOLECULAR PHYSICS*. ISSN 0026-8976, 2018, vol. 116, no. 5-6, pp. 588-601., Registrované v: WOS
 9. [1.1] PELUCCHI, M. - CAVALLOTTI, C. - FARAVELLI, T. - KLIPPENSTEIN, S. J. H-Abstraction reactions by OH, HO₂, O, O-2 and benzyl radical addition to O-2 and their implications for kinetic modelling of toluene oxidation. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 16, pp. 10607-10627., Registrované v: WOS
 10. [1.1] PENG, Bo - KOWALSKI, Karol. Green's function coupled cluster formulations utilizing extended inner excitations. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 149, no. 21, pp., Registrované v: WOS
 11. [1.1] RUSAKOV, Yury Yu - RUSAKOVA, Irina L. - SEMENOV, Valentin A. - SAMULTSEV, Dmitry O. - FEDOROV, Sergei V. - KRIVDIN, Leonid B. Calculation of N-15 and P-31 NMR Chemical Shifts of Azoles, Phospholes, and Phosphazoles: A Gateway to Higher Accuracy at Less Computational Cost. In *JOURNAL OF PHYSICAL CHEMISTRY A*. ISSN 1089-5639, 2018, vol. 122, no. 33, pp. 6746-6759., Registrované v: WOS
 12. [1.1] TAVANAEI, Leila - NORI-SHARGH, Davood. New Insights into the Origin of the cis-Configuration Preferences in 1,2-Dihaloethenes: The Importance of the Bonding Orbital Deviations. In *AUSTRALIAN JOURNAL OF CHEMISTRY*. ISSN 0004-9425, 2018, vol. 71, no. 1, pp. 1-13., Registrované v: WOS
 13. [1.1] YOKOGAWA, D. Coupled Cluster Theory Combined with Reference Interaction Site Model Self-Consistent Field Explicitly Including Spatial Electron Density Distribution. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 5, pp. 2661-2666., Registrované v: WOS
- ADCA378 VAARA, Juha - MALKINA, Olga - STOLL, H. - MALKIN, Vladimír - KAUPP, Martin. Study of relativistic effects on nuclear shieldings using density-functional theory and spin-orbit

pseudopotentials. In *Journal of Chemical Physics*, 2001, vol. 114, no. 1, p. 61-71. (2001 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] VÍCHA, Jan - KOMOROVSKÝ, Stanislav - REPISKÝ, Michal - MAREK, Radek - STRAKA, Michal. *Relativistic Spin-Orbit Heavy Atom on the Light Atom NMR Chemical Shifts: General Trends Across the Periodic Table Explained*. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 6, pp. 3025-3039., Registrované v: WOS
- ADCA379 VALERIO, G. - GOURSOT, A. - VETRIVEL, R. - MALKINA, Olga - MALKIN, Vladimír - SALAHUB, Dennis R. Calculation of ²⁹Si and ²⁷Al MAS NMR chemical shifts in zeolite-β using density functional theory: Correlation with lattice structure. In *Journal of the American Chemical Society*, 1998, vol. 120, no. 44, p. 11426-11431. ISSN 0002-7863.

Citácie:

1. [1.1] HOLMES, Sean T. - BAI, Shi - IULIUCCI, Robbie J. - MUELLER, Karl T. - DYBOWSKI, Cecil. *Calculations of Solid-State Ca-43 NMR Parameters: A Comparison of Periodic and Cluster Approaches and an Evaluation of DFT Functionals*. In *JOURNAL OF COMPUTATIONAL CHEMISTRY*. ISSN 0192-8651, 2017, vol. 38, no. 13, pp. 949-956., Registrované v: WOS
2. [1.1] JO, Changbum - PARK, Woojin - RYOO, Ryong. *Synthesis of mesoporous zeolites in fluoride media with structure directing multiammonium surfactants*. In *MICROPOROUS AND MESOPOROUS MATERIALS*. ISSN 1387-1811, 2017, vol. 239, no., pp. 19-27., Registrované v: WOS
3. [1.1] JOSEPHSON, Tyler R. - JENNESS, Glen R. - VLACHOS, Dionisios G. - CARATZOULAS, Stavros. *Distribution of open sites in Sn-Beta zeolite*. In *MICROPOROUS AND MESOPOROUS MATERIALS*. ISSN 1387-1811, 2017, vol. 245, no., pp. 45-50., Registrované v: WOS
4. [1.1] OTOMO, Ryoichi - NISHITOBA, Toshiki - OSUGA, Rota - KUNITAKE, Yusuke - KAMIYA, Yuichi - TATSUMI, Takashi - YOKOI, Toshiyuki. *Determination of Acid Site Location in Dealuminated MCM-68 by Al-27 MQMAS NMR and FT-IR Spectroscopy with Probe Molecules*. In *JOURNAL OF PHYSICAL CHEMISTRY C*. ISSN 1932-7447, 2018, vol. 122, no. 2, pp. 1180-1191., Registrované v: WOS
5. [1.1] SZELESZCZUK, Lukasz - PISKLAK, Dariusz Maciej - ZIELINSKA-PISKLAK, Monika. *Does the choice of the crystal structure influence the results of the periodic DFT calculations? A case of glycine alpha polymorph GIPAW NMR parameters computations*. In *JOURNAL OF COMPUTATIONAL CHEMISTRY*. ISSN 0192-8651, 2018, vol. 39, no. 14, pp. 853-861., Registrované v: WOS
6. [1.1] WANG, Hanlu - DENG, YiQiang - ZHOU, Rujin. *Aromatic sulfur compounds oxidation with H₂O₂ over fully coordinated and defect sites in Ti-beta zeolites: evaluation by density functional theory*. In *THEORETICAL CHEMISTRY ACCOUNTS*. ISSN 1432-881X, 2018, vol. 137, no. 5, pp., Registrované v: WOS
7. [1.1] WHITTLETON, Sarah R. - VICENTE, Aurelie - FERNANDEZ, Christian - RASTEGAR, Somayeh F. - FISHCHUK, Anna V. - SKLENAK, Stepan. *Effect of Ge/Si substitutions on the local geometry of Si framework sites in zeolites: A combined high resolution Si-29 MAS NMR and DFT/MM study on zeolite Beta polymorph C (BEC)*. In *MICROPOROUS AND MESOPOROUS MATERIALS*. ISSN 1387-1811, 2018, vol. 267, no., pp. 124-133., Registrované v: WOS

- ADCA380 VALIRON, Pierre - WERNLI, Michael - FAURE, Alexandre - WIESENFELD, Laurent - RIST, Claire - KEDŽUCH, Stanislav - NOGA, Jozef. R12-calibrated H₂O-H₂ interaction: Full dimensional and vibrationally averaged potential energy surfaces. In *Journal of Chemical Physics*, 2008, vol. 129, no. 13, p. 134306-1-134306-14. (2007: 3.044 - IF, karentované - CCC). (2008 - Current Contents). ISSN 0021-9606.

Citácie:

1. [1.1] BENOIT, David M. - LAUVERGNAT, David - SCRIBANO, Yohann. *Does cage quantum delocalisation influence the translation-rotational bound states of molecular hydrogen in clathrate hydrate?* In *FARADAY DISCUSSIONS*. ISSN 1359-6640, 2018, vol. 212, no., pp. 533-546., Registrované v: WOS
 2. [1.1] BORYSOW, Jacek - MORALDI, Massimo - NEUMANN, Martin. *Calculation of the Raman Q branch of hydrogen in water and comparison with experiments*. In *JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS*. ISSN 0953-4075, 2018, vol. 51, no. 23, pp., Registrované v: WOS
 3. [1.1] POWERS, Anna - SCRIBANO, Yohann - LAUVERGNAT, David - MEBE, Elsy - BENOIT, David M. - BACIC, Zlatko. *The effect of the condensed-phase environment on the vibrational frequency shift of a hydrogen molecule inside clathrate hydrates*. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 14, pp., Registrované v: WOS
 4. [1.1] ZHANG, Xiao-Long - MA, Yong-Tao - ZHAI, Yu - LI, Hui. *Analytic Morse/long-range potential energy surfaces and "adiabatic-hindered-rotor" treatment for a symmetric top-linear molecule dimer: A case study of CH₃F-H-2*. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 12, pp., Registrované v: WOS
- ADCA381 VALÚCHOVÁ, Jana - MADEJOVÁ, Jana - KOMADEL, Peter. Effect of heating temperature on Li-fixation, layer charge and properties of fine fractions of bentonites. In *Journal of Materials Chemistry*, 2001, vol. 11, no. 5, p. 1452-1457. ISSN 0959-9428.

Citácie:

1. [1.1] BODART, Philippe R. - DELMOTTE, L. - RIGOLET, S. - BRENDLE, J. - GOUGEON, Regis D. *Li-7{F-19} TEDOR NMR to observe the lithium migration in heated montmorillonite*. In *APPLIED CLAY SCIENCE*. ISSN 0169-1317, 2018, vol. 157, no., pp. 204-211., Registrované v: WOS
 2. [1.1] WANG, Wei - ZHAO, Yunliang - YI, Hao - CHEN, Tianxing - KANG, Shichang - LI, Hongqiang - SONG, Shaoxian. *Preparation and characterization of self-assembly hydrogels with exfoliated montmorillonite nanosheets and chitosan*. In *NANOTECHNOLOGY*. ISSN 0957-4484, 2018, vol. 29, no. 2, pp., Registrované v: WOS
- ADCA382 VASKOVÁ, Zuzana - KONTRÍK, Martin - MLYNÁRIKOVÁ, Jarmila - BOČA, Miroslav. Density of

low-temperature KF-AlF₃ aluminum baths with Al₂O₃ and AlPO₄ additives. In *Metallurgical and Materials Transactions B : Process Metallurgy and Materials Processing Science*, 2015, vol. 46, no. 1, p. 485-493. (2014: 1.461 - IF, Q1 - JCR, 1.042 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents). ISSN 1073-5615.

Citácie:

1. [1.1] KUBINAKOVA, Emilia - DANIELIK, Vladimir - HIVES, Jan. *Electrical Conductivity of Low-Temperature Potassium Cryolite Electrolytes Suitable for Innovation of Aluminum Preparation*. In *JOURNAL OF THE ELECTROCHEMICAL SOCIETY*. ISSN 0013-4651, 2018, vol. 165, no. 7, pp. E274-E278., Registrované v: WOS

ADCA383 VASKOVÁ, Zuzana - KITANOVSKI, Nives - JAGLIČIĆ, Zvonko - STRAUCH, Peter - RŮŽIČKOVÁ, Zdeňka - VALIGURA, D. - KOMAN, M. - KOZLEVČAR, Bojan - MONCOL, J. Synthesis and magneto-structural characterization of copper(II) nitrobenzoate complexes containing nicotinamide or methyl nicotinamide ligands. In *Polyhedron*, 2014, vol. 81, p. 555-563. (2013: 2.047 - IF, 0.548 - SJR, karentované - CCC). (2014 - Current Contents). ISSN 0277-5387.

Citácie:

1. [1.1] SANCHEZ-SALA, Marta - PONS, Josefina - ALVAREZ-LARENA, Angel - BAYES-GARCIA, Laura - FONT-BARDIA, Merce - AYLLON, Jose A. *Cu(II) 4-phenoxybenzoate dimers and monomer coordinated by pyridines: Synthesis and crystal structures*. In *POLYHEDRON*. ISSN 0277-5387, 2018, vol. 151, no., pp. 545-553., Registrované v: WOS

ADCA384 VÍCHA, Jan - KOMOROVSKÝ, Stanislav - REPISKÝ, Michal - MAREK, Radek - STRAKA, Michal. Relativistic spin-orbit heavy atom on the light atom NMR chemical shifts: General trends across the periodic table explained. In *Journal of Chemical Theory and Computation*, 2018, vol. 14, no. 6, p. 3025-3039. (2017: 5.399 - IF, Q1 - JCR, 2.497 - SJR, Q1 - SJR, karentované - CCC). (2018 - Current Contents). ISSN 1549-9618.

Citácie:

1. [1.1] FIELD-THEODORE, Terri E. - OLEJNICZAK, Malgorzata - JASZUNSKI, Michal - WILSON, David J. D. *NMR shielding constants in group 15 trifluorides*. In *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*. ISSN 1463-9076, 2018, vol. 20, no. 35, pp. 23025-23033., Registrované v: WOS

ADCA385 WEBB, Jeffrey A. - LIU, Pei-Hua - MALKINA, Olga - GOROFF, Nancy S. Tetraiodobutatriene: A new cumulenenic carbon iodide. In *Angewandte Chemie*, 2002, vol. 41, no. 16, p. 3011-3014. ISSN 1433-7851.

Citácie:

1. [1.1] BRUCE, Michael I. - HEAD, Nicholas J. - SKELTON, Brian W. - SPACKMAN, Mark A. - WHITE, Allan H. *Tetraiodoallene, I₂C = C = CI₂ the missing link between I₂C = CI₂ and I₂C = C = C = CI₂ and the oxidation product, 2,2-diiodoacrylic acid, I₂C = CH(CO₂H)*. In *AUSTRALIAN JOURNAL OF CHEMISTRY*. ISSN 0004-9425, 2018, vol. 71, no. 1, pp. 70-73., Registrované v: WOS

ADCA386 YADAV, S. - KUŘITKA, Ivo - HAVLICA, Jaromír - HNATKO, Miroslav - CIGÁŇ, Alexander - MASILKO, J. - KALINA, L. - HAJDÚCHOVÁ, M. - RUSNÁK, Jaroslav - ENEV, V. Structural, magnetic, elastic, dielectric and electrical properties of hot-pressed sintered Co_{1-x}Zn_xFe₂O₄ (x = 0.0, 0.5) spinel ferrite nanoparticles. In *Journal of Magnetism and Magnetic Materials*, 2018, vol. 447, p. 48-57. (2017: 3.046 - IF, Q2 - JCR, 0.786 - SJR, Q1 - SJR, karentované - CCC). (2018 - Current Contents, WOS, SCOPUS). ISSN 0304-8853.

Citácie:

1. [1.1] ATI, Ali A. *Fast synthesis, structural, morphology with enhanced magnetic properties of cobalt doped nickel ferrite nanoscale*. In *JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS*. ISSN 0957-4522, 2018, vol. 29, no. 14, pp. 12010-12021., Registrované v: WOS

2. [1.1] PHAM HOAI LINH - NGUYEN THI NGOC ANH - PHAM HONG NAM - TA NGOC BACH - VU DINH LAM - DO HUNG MANH. *A Facile Ultrasound Assisted Synthesis of Dextran-Stabilized Co_{0.2}Fe_{0.8}Fe₂O₄ Nanoparticles for Hyperthermia Application*. In *IEEE TRANSACTIONS ON MAGNETICS*. ISSN 0018-9464, 2018, vol. 54, no. 6., Registrované v: WOS

ADCA387 YADAV, S. - HAVLICA, J. - HNATKO, Miroslav - ŠAJGALÍK, Pavol - CIGÁŇ, Alexander - PALOU, M. - BARTONÍČKOVÁ, E. - BOHÁČ, M. - FRAJKOROVÁ, F. - MASILKO, J. - ZMRZLÝ, M. - KALINA, L. - HAJDÚCHOVÁ, M. - ENEV, V. Magnetic properties of Co_{1-x}Zn_xFe₂O₄ spinel ferrite nanoparticles synthesized by starch-assisted sol-gel autocombustion method and its ball milling. In *Journal of Magnetism and Magnetic Materials*, 2015, vol. 378, p. 190-199. (2014: 1.970 - IF, Q2 - JCR, 0.821 - SJR, Q1 - SJR, karentované - CCC). (2015 - Current Contents, WOS, SCOPUS). ISSN 0304-8853.

Citácie:

1. [1.1] ABRAIME, B. - MAHMOUD, A. - BOSCHINI, F. - TAMERD, M. Ait - BENYOUSSEF, A. - HAMEDOUN, M. - XIAO, Y. - EL KENZ, A. - MOUNKACHI, O. *Tunable maximum energy product in CoFe₂O₄ nanopowder for permanent magnet application*. In *JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS*. ISSN 0304-8853, 2018, vol. 467, pp. 129-134., Registrované v: WOS

2. [1.1] ALBURQUENQUE, D. - DENARDIN, J. C. - TRONCOSO, L. - MARCO, J. F. - GAUTIER, J. L. *Substitution effects on the bulk and surface properties of (Li,Ni)Mn₂O₄*. In *IONICS*. ISSN 0947-7047, 2018, vol. 24, no. 4, pp. 977-

- 987., Registrované v: WOS
3. [1.1] BHAME, Shekhar D. - JOY, P. A. Enhanced strain sensitivity in magnetostrictive spinel ferrite $\text{Co}_{1-x}\text{Zn}_x\text{Fe}_2\text{O}_4$. In *JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS*. ISSN 0304-8853, 2018, vol. 447, pp. 150-154., Registrované v: WOS
 4. [1.1] BROMHO, Tapos Kumar - IBRAHIM, Khalil - KABIR, Humayun - RAHMAN, M. Mahbubur - HASAN, Kamrul - FERDOUS, Tahmina - TAHA, Hatem - ALTARAWNEH, Mohammednoor - JIANG, Zhong-Tao. Understanding the impacts of Al³⁺-substitutions on the enhancement of magnetic, dielectric and electrical behaviors of ceramic processed nickel-zinc mixed ferrites: FTIR assisted studies. In *MATERIALS RESEARCH BULLETIN*. ISSN 0025-5408, 2018, vol. 97, pp. 444-451., Registrované v: WOS
 5. [1.1] CARP, Oana. Carbohydrate based combustion synthesis: A promise of greening materials synthesis. In *REVUE ROUMAINE DE CHIMIE*. ISSN 0035-3930, 2018, vol. 63, no. 9, pp. 795., Registrované v: WOS
 6. [1.1] CHAI, Zhengjun - TAN, Guoqiang - YUE, Zhongwei - XUE, Mintao - LIU, Yun - LV, Long - REN, Huijun - XIA, Ao. Structural transition, defect complexes and improved ferroelectric behaviors of $\text{Bi}_{0.88}\text{Sr}_{0.03}\text{Gd}_{0.09}\text{Fe}_{0.94}\text{Mn}_{0.04}\text{Co}_{0.02}\text{O}_3/\text{Co}_{1-x}\text{Mn}_x\text{Fe}_2\text{O}_4$ bilayer thin films. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 13, pp. 15770-15777., Registrované v: WOS
 7. [1.1] ELSHAHAWY, Abdelnaby Mohamed - MAKHLOUF, Salah Ahmed. Structural and Magnetization Studies of Cobalt Ferrite Nanoparticles Synthesized by the Microwave-Combustion Method. In *CURRENT ANALYTICAL CHEMISTRY*. ISSN 1573-4110, 2018, vol. 14, no. 6, pp. 641-645., Registrované v: WOS
 8. [1.1] GABAL, M. A. - AL-JUAID, A. A. - EL-RASHED, S. - HUSSEIN, M. A. - AL ANGARI, Y. M. Polyaniline/ $\text{Co}_{0.6}\text{Zn}_{0.4}\text{Fe}_2\text{O}_4$ core-shell nano-composites. Synthesis, characterization and properties. In *JOURNAL OF ALLOYS AND COMPOUNDS*. ISSN 0925-8388, 2018, vol. 747, pp. 83-90., Registrované v: WOS
 9. [1.1] KUBISZTAL, M. - KUBISZTAL, J. - KAROLUS, M. - PRUSIK, K. - HANECZOK, G. Evolution of frozen magnetic state in co-precipitated $\text{Zn}_{\delta}\text{Co}_{1-\delta}\text{Fe}_2\text{O}_4$ ($0 \leq \delta \leq 1$) ferrite nanopowders. In *JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS*. ISSN 0304-8853, 2018, vol. 454, pp. 368-374., Registrované v: WOS
 10. [1.1] MALEKI, Ali - HOSSEINI, Nazanin - TAHERIZADEH, AliReza. Synthesis and characterization of cobalt ferrite nanoparticles prepared by the glycine-nitrate process. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 7, pp. 8576-8581., Registrované v: WOS
 11. [1.1] PEYMANFAR, Reza - RAHMANISAGHIEH, Mitra. Preparation of neat and capped BaFe_2O_4 nanoparticles and investigation of morphology, magnetic, and polarization effects on its microwave and optical performance. In *MATERIALS RESEARCH EXPRESS*. ISSN 2053-1591, 2018, vol. 5, no. 10., Registrované v: WOS
 12. [1.1] POWAR, Rohit R. - PHADTARE, Varsha D. - PARALE, Vinayak G. - PARK, Hyung-Ho - PATHAK, Sachin - KAMBLE, Pravin R. - PISTE, Pravina B. - ZAMBARE, Dnyanashwar N. Structural, morphological, and magnetic properties of $\text{Zn}_x\text{Co}_{1-x}\text{Fe}_2\text{O}_4$ ($0 \leq x \leq 1$) prepared using a chemical co-precipitation method. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 17, pp. 20782-20789., Registrované v: WOS
 13. [1.1] PRASAD, B. B. V. S. Vara - RAMESH, K. V. - SRINIVAS, Adiraj. Structural and Soft Magnetic Properties of Nickel-Substituted Co-Zn Nanoferrites. In *JOURNAL OF SUPERCONDUCTIVITY AND NOVEL MAGNETISM*. ISSN 1557-1939, 2018, vol. 31, no. 10, pp. 3223-3237., Registrované v: WOS
 14. [1.1] PRASAD, B. B. V. S. Vara - RAMESH, K. V. - SRINIVAS, Adiraj. Structural, morphological and magnetic properties of divalent copper-substituted Co-Zn Nanoferrites. In *INTERNATIONAL JOURNAL OF MODERN PHYSICS B*. ISSN 0217-9792, 2018, vol. 32, no. 14., Registrované v: WOS
 15. [1.1] SAGAYARAJ, R. - ARAVAZHI, S. - CHANDRASEKARAN, G. Synthesis, Spectroscopy, and Magnetic Characterizations of PVP-Assisted Nanoscale Particle. In *JOURNAL OF SUPERCONDUCTIVITY AND NOVEL MAGNETISM*. ISSN 1557-1939, 2018, vol. 31, no. 10, pp. 3379-3386., Registrované v: WOS
 16. [1.1] TAN, Guoqiang - CHAI, Zhengjun - ZHENG, Yujuan - YUE, Zhongwei - REN, Huijun - XIA, Ao - YANG, Wei - LV, Long - XUE, Mintao - LIU, Yun. Resistive switching behavior and improved multiferroic properties of $\text{Bi}_{0.9}\text{Er}_{0.1}\text{Fe}_{0.98}\text{Co}_{0.02}\text{O}_3/\text{Co}_{1-x}\text{Mn}_x\text{Fe}_2\text{O}_4$ bilayered thin films. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 11, pp. 12600-12609., Registrované v: WOS
 17. [1.1] TAN, Guoqiang - CHAI, Zhengjun - ZHENG, Yujuan - YUE, Zhongwei - YANG, Wei - GUO, Meiyu - REN, Huijun - XIA, Ao - LV, Long - LIU, Yun. Tunable structural transition and multiferroic properties of the composite thin films through the structural transition of magnetic layer. In *JOURNAL OF THE EUROPEAN CERAMIC SOCIETY*. ISSN 0955-2219, 2018, vol. 38, no. 13, pp. 4463-4475., Registrované v: WOS
 18. [1.2] GABAL, M. A. - AL-ZAHRANI, N. H. - AL ANGARI, Y. M. - SAAED, A. Substitution effect on the structural, magnetic, and electrical properties of $\text{Co}_{1-x}\text{Zn}_x\text{Fe}_2\text{O}_4$ nanocrystalline ferrites ($x = 0-1$) prepared via gelatin auto-combustion method. In *IEEE Transactions on Magnetics*. ISSN 0018-9464, 2018, vol. 54, no. 1., Registrované v: SCOPUS
 19. [1.2] MOHAMMED, M. A. - SUDIN, Izman - NOOR, Alias Mohd - RAJOO, Srithar - UDAY, M. B. - OBAYES, Noor H. - OMAR, Muhammad Firdaus. Investigation on microstructure and electrical properties of Bi doping $\text{Ca}_3\text{Co}_4\text{O}_9$ nanoparticles synthesized by solgel process. In *International Journal of Engineering and Technology(UAE)*, 2018, vol. 7, no. 2, pp. 31-33., Registrované v: SCOPUS
- ADCA388 YAU, Bao-Shun - HUANG, J.-L. - LU, Horng-Hwa - ŠAJGALÍK, Pavol. Investigation of nanocrystal-
($\text{Ti}_{1-x}\text{Al}_x$)N-y/amorphous- Si_3N_4 nanolaminate films. In *Surface and coatings technology*, 2005, vol. 194, no. 1, p. 119-127. ISSN 0257-8972.

Citácie:

1. [1.1] DU JUN - ZHU XIAO-YING - WANG HONG-MEI. Nano Multilayer Structure Toughening of Hard Coatings-Method, Mechanism and Application. In CAILIAO GONGCHENG-JOURNAL OF MATERIALS ENGINEERING. ISSN 1001-4381, 2017, vol. 45, no. 8, pp. 102-114., Registrované v: WOS

2. [1.1] SUI, Xudong - LI, Guojian - JIANG, Chenjie - WANG, Kai - ZHANG, Yingjie - HAO, Junying - WANG, Qiang. Improved toughness of layered architecture TiAlN/CrN coatings for titanium high speed cutting. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 5, pp. 5629-5635., Registrované v: WOS

ADCA389 YAU, Bao-Shun - HUANG, J.-L. - LII, Ding-Fwu - ŠAJGALÍK, Pavol. Investigation of nanocrystal-(Ti,Al)N-x/amorphous-SiN_y composite films by co-deposition process. In Surface and coatings technology, 2004, vol. 177-178, p. 209-214. ISSN 0257-8972.

Citácie:

1. [1.1] TAN, Chaolin - ZHOU, Kesong - KUANG, Tongchun - LI, Yuling - MA, Wenyu. Novel performances of in situ plasma nitriding-PVD duplex-treated nanocrystalline TiN coatings. In SURFACE ENGINEERING. ISSN 0267-0844, 2018, vol. 34, no. 7, pp. 520-526., Registrované v: WOS

2. [1.1] WANG EN-QING - YUE JIAN-LING - LI MIAO-LEI - LI DONG - HUANG FENG. Influence of Si Content on Microstructure, Mechanical Properties and Tribological Properties of VAlSiN Coatings. In CAILIAO GONGCHENG-JOURNAL OF MATERIALS ENGINEERING. ISSN 1001-4381, 2017, vol. 45, no. 4, pp. 70-76., Registrované v: WOS

ADCA390 YAZYEV, Oleg V. - HELM, Lothar - MALKIN, Vladimír - MALKINA, Oľga. Quantum chemical investigation of hyperfine coupling constants on first coordination sphere water molecule of gadolinium(III) aqua complexes. In Journal of Physical Chemistry A.Molecules, spectroscopy, kinetics, environment, and general theory, 2005, vol. 109, no. 48, p. 10997-11005. ISSN 1089-5639.

Citácie:

1. [1.1] KHAN, S. - PETERS, V. - KOWALEWSKI, J. - ODELIUS, M. Zero-field splitting in the isoelectronic aqueous Gd(III) and Eu(II) complexes from a first principles analysis. In CHEMICAL PHYSICS. ISSN 0301-0104, 2018, vol. 503, no., pp. 56-64., Registrované v: WOS

2. [1.1] LINO, Jessica B. dos R. - RAMALHO, Teodorico C. Quantum Information and Nuclear Magnetic Resonance Parameters. In REVISTA VIRTUAL DE QUIMICA. ISSN 1984-6835, 2018, vol. 10, no. 4, pp. 940-962., Registrované v: WOS

ADCA391 ZAHN, G. - GROSMANN, G. - SCHELLER, D. - MALKINA, Oľga. Polymorphie von Bis(dineopentoxophosphorothioyl)diselenid - Korrelation von Röntgenstruktur und MAS-NMR-Daten = Polymorphism of bis(dineopentoxophosphorothioyl)diselenide - Correlation of X-ray structure and MAS NMR data. In Zeitschrift für anorganische und allgemeine chemie, 2000, vol. 626, no. 2, p. 524-528.

Citácie:

1. [1.1] ARTEM';EV, Alexander V. - DORONINA, Evgeniya P. - BAGRYANSKAYA, Irina Yu - KLYBA, Lyudmila V. Bis(dicyclohexylselenophosphinyl)selenide, [Cy₂P(Se)](2)Se: Synthesis, molecular structure and application for self-assembly of a tetrahedral Cu(I) cluster. In JOURNAL OF MOLECULAR STRUCTURE. ISSN 0022-2860, 2018, vol. 1160, no., pp. 208-214., Registrované v: WOS

ADCA392 ZEMANOVÁ, Matilda - LECOMTE, E. - ŠAJGALÍK, Pavol - RIEDEL, Ralf. Polysilazane derived micro/nano Si₃N₄/SiC composites. In Journal of the European Ceramic Society, 2002, vol. 22, no. 16, p. 2963-2968. ISSN 0955-2219.

Citácie:

1. [1.1] LIGON, S. Clark - BLUGAN, Gurdial - DALCANALE, Federico - KUEBLER, Jakob. Production of improved SiC and SiCN ceramics from polycarbosilane and polysilazane composites. In 9TH INTERNATIONAL CONFERENCE ON TIMES OF POLYMERS AND COMPOSITES: FROM AEROSPACE TO NANOTECHNOLOGY. ISSN 0094-243X, 2018, vol. 1981, no., pp., Registrované v: WOS

ADCA393 ZHOU, You - YOSHIZAWA, Yu-ichi - HIRAO, Kiyoshi - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol. Combustion synthesis of LaSi₃N₅:Eu²⁺ phosphor powders. In Journal of the European Ceramic Society, 2011, vol. 31, no. 1-2, p. 151-157. (2010: 2.574 - IF, karentované - CCC). (2011 - Current Contents, WOS, SCOPUS). ISSN 0955-2219.

Citácie:

1. [1.1] TEN KATE, Otmar M. - ZHANG, Zhijun - VAN OMMEN, J. Ruud - HINTZEN, H. T. (Bert). Dependence of the photoluminescence properties of Eu²⁺-doped M- Si- N (M = alkali, alkaline earth or rare earth metal) nitridosilicates on their structure and composition. In JOURNAL OF MATERIALS CHEMISTRY C. ISSN 2050-7526, 2018, vol. 6, no. 21, pp. 5671-5683., Registrované v: WOS

2. [1.1] WANG, Shuxin - SONG, Zhen - KONG, Yuwei - XIA, Zhiguo - LIU, Quanlin. Crystal field splitting of 4f(n-1)5d-levels of Ce³⁺ and Eu²⁺ in nitride compounds. In JOURNAL OF LUMINESCENCE. ISSN 0022-2313, 2018, vol. 194, no., pp. 461-466., Registrované v: WOS

ADCA394 ZHOU, You - YOSHIZAWA, Yu-ichi - HIRAO, Kiyoshi - LENČEŠ, Zoltán - ŠAJGALÍK, Pavol. Preparation of Eu-doped beta-SiAlON phosphors by combustion synthesis. In Journal of the American Ceramic Society, 2008, vol. 91, no. 9, p. 3082-3085. (2007: 1.792 - IF, karentované - CCC). (2008 - Current Contents). ISSN 0002-7820.

Citácie:

1. [1.1] LIU QIAN - ZHOU ZHEN-ZHEN. Progress in Activated-synthesis of Si-based Oxynitrides Materials at Low Temperatures. In JOURNAL OF INORGANIC MATERIALS. ISSN 1000-324X, 2018, vol. 33, no. 2, pp. 129-137., Registrované v: WOS
 2. [1.1] LOHE, P. P. - NANDANWAR, D. V. - BELSARE, P. D. - MOHARIL, S. V. Recent Developments in White Light Emitting Diodes. In 2ND INTERNATIONAL CONFERENCE ON CONDENSED MATTER AND APPLIED PHYSICS (ICC-2017). ISSN 0094-243X, 2018, vol. 1953, no., pp., Registrované v: WOS
- ADCA395 ZHOU, You - ZHU, Xinwen - HIRAO, Kiyoshi - LENČEŠ, Zoltán. Sintered reaction-bonded silicon nitride with high thermal conductivity and high strength. In International Journal of Applied Ceramic Technology, 2008, vol. 5, no. 2, p. 119-126. ISSN 1744-7402.
- Citácie:
1. [1.1] HYUGA, Hideki. Development of efficient fabrication processes for highly functional silicon nitride ceramics: a review. In JOURNAL OF THE CERAMIC SOCIETY OF JAPAN. ISSN 1882-0743, 2018, vol. 126, no. 12, pp. 968-976., Registrované v: WOS
- ADCA396 ZHU, Xinwen - ZHOU, You - HIRAO, Kiyoshi - LENČEŠ, Zoltán. Processing and thermal conductivity of sintered reaction-bonded silicon nitride: (I) Effect of Si powder characteristics. In Journal of the American Ceramic Society, 2006, vol. 89, no. 11, p. 3331-3339. (2005: 1.586 - IF, karentované - CCC). (2006 - Current Contents). ISSN 0002-7820.
- Citácie:
1. [1.1] DUAN, Yusen - ZHANG, Jingxian - LI, Xiaoguang - SHI, Ying - XIE, Jianjun - JIANG, Dongliang. Low temperature pressureless sintering of silicon nitride ceramics for circuit substrates in powder electronic devices. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 4, pp. 4375-4380., Registrované v: WOS
 2. [1.1] GO, Shin-Il - LI, Yinsheng - KO, Jae-Woong - KIM, Ha-Neul - KWON, Se-Hun - KIM, Hai-Doo - PARK, Young-Jo. Microstructure and Thermal Conductivity of Sintered Reaction-Bonded Silicon Nitride: The Particle Size Effects of MgO Additive. In ADVANCES IN MATERIALS SCIENCE AND ENGINEERING. ISSN 1687-8434, 2018, vol., no., pp., Registrované v: WOS
 3. [1.1] HYUGA, Hideki. Development of efficient fabrication processes for highly functional silicon nitride ceramics: a review. In JOURNAL OF THE CERAMIC SOCIETY OF JAPAN. ISSN 1882-0743, 2018, vol. 126, no. 12, pp. 968-976., Registrované v: WOS
 4. [1.1] JIA HONGSHENG - LI JIAQI - NIU RUI - YE CHAOCHAO - RU HONGQIANG - LIU BAOCHANG - YUANLONG, E. - LI HAIBO. Fabrication of beta-Si₃N₄ with high thermal conductivity under ultra-high pressure. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 18, pp. 23288-23292., Registrované v: WOS
 5. [1.1] LOGESH, G. - RASHAD, Mohammed - LODHE, Mangesh - SABU, Ummen - JOSEPH, Andrews - RAJU, K. C. James - BALASUBRAMANIAN, M. Mechanical and dielectric properties of carbon fiber reinforced reaction bonded silicon nitride composites. In JOURNAL OF ALLOYS AND COMPOUNDS. ISSN 0925-8388, 2018, vol. 767, no., pp. 1083-1093., Registrované v: WOS
 6. [1.1] MINASYAN, Tatevik - LIU, Le - AGHAYAN, Marina - KOLLO, Lauri - KAMBOJ, Nikhil - AYDINYAN, Softiya - HUSSAINOVA, Irina. A novel approach to fabricate Si₃N₄ by selective laser melting. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 12, pp. 13689-13694., Registrované v: WOS
 7. [1.1] MORITA, Seitaro - IJIMA, Motoyuki - TATAMI, Junichi. Microstructural control of green bodies prepared from Si-based multi-component non-aqueous slurries and their effects on fabrication of Si₃N₄ ceramics through post-reaction sintering. In ADVANCED POWDER TECHNOLOGY. ISSN 0921-8831, 2018, vol. 29, no. 12, pp. 3199-3209., Registrované v: WOS
 8. [1.1] YANG, Chunping - YE, Feng - MA, Jie - DING, Junjie - ZHANG, Biao - LIU, Qiang - ZHANG, Haoqian. Comparative study of fluoride and non-fluoride additives in high thermal conductive silicon nitride ceramics fabricated by spark plasma sintering and post-sintering heat treatment. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 18, pp. 23202-23207., Registrované v: WOS
- ADCA397 ZIMOWSKA, Malgorzata - PÁLKOVÁ, Helena - MADEJOVÁ, Jana - DULA, Roman - PAMIN, Katarzyna - OLEJNICZAK, Zbigniew - GIL, Barbara - SERWICKA, Ewa M. Laponite-derived porous clay heterostructures: III. The effect of alumination. In Microporous and Mesoporous Materials, 2013, vol. 175, p. 67-75. (2012: 3.365 - IF, 1.489 - SJR, karentované - CCC). (2013 - Current Contents).(Vega č. 2/0183/09 : Chemické modifikácie povrchov prírodných nanomateriálov).
- Citácie:
1. [1.1] CECILIA, J. A. - GARCIA-SANCHO, C. - VILARRASA-GARCIA, E. - JIMENEZ-JIMENEZ, J. - RODRIGUEZ-CASTELLON, E. Synthesis, Characterization, Uses and Applications of Porous Clays Heterostructures: A Review. In CHEMICAL RECORD. ISSN 1527-8999, 2018, vol. 18, no. 7-8, pp. 1085-1104., Registrované v: WOS
- ADCA398 ZIMOWSKA, Malgorzata - GURGUL, J. - PÁLKOVÁ, Helena - OLEJNICZAK, Zbigniew - LATKA, K. - LITYNSKA-DOBZYNSKA, L. - MATACHOWSKI, L. Structural rearrangements in Fe-porous clay heterostructures composites derived from Laponite® - Influence of preparation methods and Fe source. In Microporous and Mesoporous Materials, 2016, vol. 231, p. 66-81. (2015: 3.349 - IF, Q1 - JCR, 1.205 - SJR, Q1 - SJR, karentované - CCC). (2016 - Current Contents). ISSN 1387-1811.
- Citácie:
1. [1.1] CECILIA, J. A. - GARCIA-SANCHO, C. - VILARRASA-GARCIA, E. - JIMENEZ-JIMENEZ, J. - RODRIGUEZ-CASTELLON, E. Synthesis, Characterization, Uses and Applications of Porous Clays Heterostructures: A Review. In

CHEMICAL RECORD. ISSN 1527-8999, 2018, vol. 18, no. 7-8, pp. 1085-1104., Registrované v: WOS
 2. [1.1] YUAN, Minhao - DENG, Wenyi - DONG, Shilin - LI, Qiancheng - ZHAO, Bingtao - SU, Yaxin. Montmorillonite based porous clay heterostructures modified with Fe as catalysts for selective catalytic reduction of NO with propylene. In CHEMICAL ENGINEERING JOURNAL. ISSN 1385-8947, 2018, vol. 353, no., pp. 839-848., Registrované v: WOS

ADCB Vedecké práce v zahraničných karentovaných časopisoch – neimpaktovaných

ADCB01 TEN-NO, Seiichiro - NOGA, Jozef. Explicitly correlated electronic structure theory from R12/F12 ansätze. In Wiley Interdisciplinary Reviews-Computational Molecular Science, 2012, vol. 2, no. 1, p. 114-125. (2012 - Current Contents).

Citácie:

1. [1.1] BARCA, Giuseppe M. J. - LOOS, Pierre-Francois. Recurrence Relations for Four-Electron Integrals Over Gaussian Basis Functions. In NOVEL ELECTRONIC STRUCTURE THEORY: GENERAL INNOVATIONS AND STRONGLY CORRELATED SYSTEMS. ISSN 0065-3276, 2018, vol. 76, no., pp. 147-165., Registrované v: WOS
2. [1.1] BAYNE, Michael G. - SCHER, Jeremy A. - ELLIS, Benjamin H. - CHAKRABORTY, Arindam. Linked-Cluster Formulation of Electron-Hole Interaction Kernel in Real-Space Representation without Using Unoccupied States. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 7, pp. 3656-3666., Registrované v: WOS
3. [1.1] CHAN, Bun - SIMMIE, John M. Barriometry an enhanced database of accurate barrier heights for gas-phase reactions. In PHYSICAL CHEMISTRY CHEMICAL PHYSICS. ISSN 1463-9076, 2018, vol. 20, no. 16, pp. 10732-10740., Registrované v: WOS
4. [1.1] KESHARWANI, Manoj K. - SYLVETSKY, Nitai - KOEHN, Andreas - TEW, David P. - MARTIN, Jan M. L. Do CCSD and approximate CCSD-F12 variants converge to the same basis set limits? The case of atomization energies. In JOURNAL OF CHEMICAL PHYSICS. ISSN 0021-9606, 2018, vol. 149, no. 15, pp., Registrované v: WOS
5. [1.1] KLAUHOHN, Sascha - KAUPP, Martin - KARTON, Amir. MVO-10: A Gas-Phase Oxide Benchmark for Localization/Delocalization in Mixed-Valence Systems. In JOURNAL OF CHEMICAL THEORY AND COMPUTATION. ISSN 1549-9618, 2018, vol. 14, no. 7, pp. 3512-3523., Registrované v: WOS
6. [1.1] LASAR, Christian - KLUENER, Thorsten. Explicitly correlated orbital optimized contracted pair correlation methods: Foundations and applications. In JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY. ISSN 0219-6336, 2018, vol. 17, no. 4, pp., Registrované v: WOS
7. [1.1] MA, Qianli - WERNER, Hans-Joachim. Explicitly correlated local coupled-cluster methods using pair natural orbitals. In WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE. ISSN 1759-0876, 2018, vol. 8, no. 6, pp., Registrované v: WOS
8. [1.1] ZHAO, Yan - XIA, Lixue - LIAO, Xiaobin - HE, Qiu - ZHAO, Maria X. - TRUHLAR, Donald G. Extrapolation of high-order correlation energies: the WMS model. In PHYSICAL CHEMISTRY CHEMICAL PHYSICS. ISSN 1463-9076, 2018, vol. 20, no. 43, pp. 27375-27384., Registrované v: WOS

ADDA Vedecké práce v domácich karentovaných časopisoch – impaktovaných

ADDA01 ANDREJKOVIČOVÁ, Slávka - PENTRÁK, Martin - JANKOVIČ, Ľuboš - KOMADEL, Peter. Sorption of heavy metal cations on rhyolitic and andesitic bentonites from Central Slovakia. In Geologica Carpathica, 2010, vol. 61, no. 2, p. 163-171. (2009: 0.963 - IF, karentované - CCC). (2010 - Current Contents). ISSN 1335-0552.

Citácie:

1. [1.1] ZUZANA, Dankova - ZUZANA, Dakos - IVETA, Styriakova - ALEXANDRA, Bekenyiova. STUDY OF Cu(II) ADSORPTION BY BENTONITE AND FOLLOWING REGENERATION BY BIOLEACHING. In ARCHIVES FOR TECHNICAL SCIENCES. ISSN 1840-4855, 2018, vol., no. 19, pp. 45-56., Registrované v: WOS

ADDA02 ANDREJKOVIČOVÁ, Slávka - MADEJOVÁ, Jana - CZÍMEROVÁ, Adriana - GALKO, Igor - DOHRMANN, Reiner - KOMADEL, Peter. Mineralogy and chemistry of Fe-rich bentonite from the Lieskovec deposit (Central Slovakia). In Geologica Carpathica, 2006, vol. 57, no. 5, p. 371-378. (2005: 0.449 - IF, karentované - CCC). (2006 - Current Contents). ISSN 1335-0552.

Citácie:

1. [1.1] POLAK, Filip - URIK, Martin - BUJDOS, Marek - UHLIK, Peter - MATUS, Peter. Evaluation of aluminium mobilization from its soil mineral pools by simultaneous effect of Aspergillus strains'; acidic and chelating exometabolites. In JOURNAL OF INORGANIC BIOCHEMISTRY. ISSN 0162-0134, 2018, vol. 181, no., pp. 162-168., Registrované v: WOS

ADDA03 BOČA, Miroslav - KUCHARÍK, Marián - VASILJEV, Roman - DANĚK, V.. Surface tension of melts of the system KF-K₂MoO₄-SiO₂. In Chemical Papers - Chemické zvesti, 2003, vol. 57, no. 2, p. 68-72. (2003 - Current Contents). ISSN 0366-6352.

Citácie:

1. [1.1] LOCK, Simon J. - STEWART, Sarah T. - PETAEV, Michail I. - LEINHARDT, Zoe - MACE, Mia T. - JACOBSEN, Stein B. - CUK, Matija. The Origin of the Moon Within a Terrestrial Synestia. In JOURNAL OF

- GEOPHYSICAL RESEARCH-PLANETS. ISSN 2169-9097, 2018, vol. 123, no. 4, pp. 910-951., Registrované v: WOS**
 ADDA04 DANKO, Martin - MIČUŠÍK, Matej - OMASTOVÁ, Mária - BUJDAK, Juraj - CHORVÁT, Dušan Jr. Spectral characterisation of new organic fluorescent dyes with an alkoxysilane moiety and their utilisation for the labelling of layered silicates. In Chemical papers, 2013, vol. 67, no. 1, p. 18-28. (2012: 0.879 - IF, 0.301 - SJR, karentované - CCC). (2013 - Current Contents). ISSN 0366-6352.

Citácie:

1. [1.2] THIRUVASAGAM, P. Synthesis and characterization of new aromatic hydroxy acid compounds. In Bulletin of the Chemical Society of Ethiopia. ISSN 10113924, 2018-01-01, 32, 3, pp. 523-530., Registrované v: SCOPUS
 ADDA05 HRACHOVÁ, Jana - CHODÁK, Ivan - KOMADEL, Peter. Modification and characterization of montmorillonite fillers used in composites with vulcanized natural rubber. In Chemical papers, 2009, vol. 63, no. 1, p. 55-61. (2008: 0.758 - IF, karentované - CCC). (2009 - Current Contents). ISSN 0366-6352.

Citácie:

1. [1.1] BARANYAIOVA, T. - BUJDAK, J. EFFECTS OF DYE SURFACE CONCENTRATION ON THE MOLECULAR AGGREGATION OF XANTHENE DYE IN COLLOIDAL DISPERSIONS OF MONTMORILLONITE. In CLAYS AND CLAY MINERALS. ISSN 0009-8604, APR 2018, vol. 66, no. 2, p. 114-126., Registrované v: WOS
 2. [1.1] CAO, J. - WEN, N. - ZHENG, Y.Y. The preparation of calcium pimelate modified OMMT from natural Camontmorillonite and its application as beta-nucleating agent for polypropylene. In POLYMER TESTING. ISSN 0142-9418, FEB 2018, vol. 65, p. 352-359., Registrované v: WOS
 3. [1.1] RANGEL-PORRAS, G. - MONCADA-SANCHEZ, C. - ZARRAGA-NUNEZ, R. - ROMERO-TOLEDO, R. - MIRANDA-AVILES, R. Thermogravimetric characterization of tyrosine and catechol adsorbed on montmorillonite. In INSTRUMENTATION SCIENCE & TECHNOLOGY. ISSN 1073-9149, 2018, vol. 46, no. 6, p. 676-692., Registrované v: WOS
 4. [1.1] VERMISOGLIOU, E.C. - GIANNAKOPOULOU, T. - TODOROVA, N. - BOUKOS, N. - VAIMAKIS, T. - PETRIDIS, D. - TRAPALIS, C. Organoclay/Graphitic Nanoplatelets Lamellar Hybrid Composites. In JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY. ISSN 1533-4880, NOV 2018, vol. 18, no. 11, p. 7797-7803., Registrované v: WOS
 5. [1.1] VERMISOGLIOU, E.C. - GIANNAKOPOULOU, T. - TODOROVA, N. - VAIMAKIS, T. - BOUKOS, N. - PETRIDIS, D. - TRAPALIS, C. 2-Dimensional Clay/Reduced Graphene Oxide Ordered Heterostructures Dispersible in Water via a One-Step Hydrothermal Route. In JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY. ISSN 1533-4880, JUL 2018, vol. 18, no. 7, p. 4684-4691., Registrované v: WOS
 6. [1.1] YOSHIDA, T. - TASAKA, Y. - TANAKA, S. - PARK, H.J. - MURAI, Y. Rheological properties of montmorillonite dispersions in dilute NaCl concentration investigated by ultrasonic spinning rheometry. In APPLIED CLAY SCIENCE. ISSN 0169-1317, SEP 1 2018, vol. 161, p. 513-523., Registrované v: WOS
 ADDA06 ŠIMKO, František - DANĚK, V.. Cryoscopy in the system Na₃AlF₆-Fe₂O₃. In Chemical Papers - Chemické zvesti, 2001, vol. 55, no. 5, p. 269-272. ISSN 0366-6352.

Citácie:

1. [1.1] KUBIKOVA, Blanka - MLYNARIKOVA, Jarmila - BENES, Ondrej - MIKSIKOVA, Eva - PRISCAK, Jozef - TOSOLIN, Alberto - BOCA, Miroslav. Physico-chemical properties of the system (LiF-NaF)(eut)-LaF₃ Phase equilibria, density and volume properties, electrical conductivity and surface tension. In JOURNAL OF MOLECULAR LIQUIDS. ISSN 0167-7322, 2018, vol. 268, no., pp. 754-761., Registrované v: WOS

ADEA Vedecké práce v ostatných zahraničných časopisoch – impaktovaných

- ADEA01 ŽIVICA, Vladimír - BALKOVIC, Svetozár - DRÁBIK, Milan. Properties of metakaolin geopolymer hardened paste prepared by high-pressure compaction. In Construction and Building Materials, 2011, vol. 25, p. 2206-2213. (2010: 1.366 - IF). (2011 - Thomson Reuters Master Journal List). ISSN 0950-0618.

Citácie:

1. [1.1] KHALID, H. R. - LEE, N. K. - PARK, S. M. - ABBAS, N. - LEE, H. K. Synthesis of geopolymer-supported zeolites via robust one-step method and their adsorption potential. In JOURNAL OF HAZARDOUS MATERIALS. ISSN 0304-3894, 2018, vol. 353, p. 522-533., Registrované v: WOS
 2. [1.1] KHATER, H. M. - EZZAT, M. Preparation and characterization of engineered stones based geopolymer composites. In JOURNAL OF BUILDING ENGINEERING. ISSN 2352-7102, 2018, vol. 20, p. 493-500., Registrované v: WOS
 3. [1.2] EAN, L. W. - MALEK, M. A. - MOHAMMED, B. S. - TANG, C. W. - BONG, P. X. H. A review on characterization of sediments for Green bricks production. In International Journal of Engineering and Technology(UAE), 2018, 7, 4, p. 41-47., Registrované v: SCOPUS

ADEB Vedecké práce v ostatných zahraničných časopisoch – neimpaktovaných

- ADEB01 GALLO, Jiří - STEWART, Todd - NOVOTNÝ, Radek - DUSZA, Ján - GALUSEK, Dušan. Early fracture of a plasma cup ceramic liner: a case report and surface analysis. In Biomedical Papers, 2007,

vol. 151, no. 2, p. 341-346. ISSN 1213-8118.

Citácie:

1. [1.1] CUCCHI, Davide - GATHEN, Martin - STREICHER, Robert - WIRTZ, Dieter Christian. *Ceramic-on-Ceramic in Total Hip Replacement Revision*. In *Zeitschrift für Orthopädie und Unfallchirurgie*. ISSN 18646697, 2018-01-01, 156, 3, pp. 272-280., Registrované v: WOS

ADEB02 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.

Citácie:

1. [1.1] FOPPA, Lucas - YAMAMOTO, Keishi - LIAO, Wei-Chih - COMAS-VIVES, Aleix - COPERET, Christophe. *Electronic Structure-Reactivity Relationship on Ruthenium Step-Edge Sites from Carbonyl C-13 Chemical Shift Analysis*. In *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*. ISSN 1948-7185, 2018, vol. 9, no. 12, pp. 3348-3353., Registrované v: WOS

ADEB03 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.

Citácie:

1. [1.1] CUNY, Jerome - JOLIBOIS, Franck - GERBER, Iann C. *Evaluation of Gas-to-Liquid O-17 Chemical Shift of Water: A Test Case for Molecular and Periodic Approaches*. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*. ISSN 1549-9618, 2018, vol. 14, no. 8, pp. 4041-4051., Registrované v: WOS

2. [1.1] GALAMBA, N. - CABRAL, Benedito J. C. *Magnetic properties and core electron binding energies of liquid water*. In *JOURNAL OF CHEMICAL PHYSICS*. ISSN 0021-9606, 2018, vol. 148, no. 4, pp., Registrované v: WOS

3. [1.1] YESILTEPE, Yasemin - NUNEZ, Jamie R. - COLBY, Sean M. - THOMAS, Dennis G. - BORKUM, Mark I. - REARDON, Patrick N. - WASHTON, Nancy M. - METZ, Thomas O. - TEEGUARDEN, Justin G. - GOVIND, Niranjan - RENSLOW, Ryan S. *An automated framework for NMR chemical shift calculations of small organic molecules*. In *JOURNAL OF CHEMINFORMATICS*. ISSN 1758-2946, 2018, vol. 10, no., pp., Registrované v: WOS

ADEB04 TATARKO, Peter - LOJANOVÁ, Š. - DUSZA, Ján - ŠAJGALÍK, Pavol. *Characterization of rare-earth doped Si₃N₄/SiC micro/nano-composites*. In *Processing and Application of Ceramics*, 2010, vol. 4, no. 1, p. 25-32.

Citácie:

1. [1.1] LI, Bin - LI, Guangqi - CHEN, Haiyang - CHEN, Junhong - HOU, Xinmei - LI, Yong. *Reaction and formation mechanism of Fe-Si₃N₄ composite prepared by flash combustion synthesis*. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 18, pp. 22777-22783., Registrované v: WOS

2. [1.1] LI, Bin - LI, Guangqi - CHEN, Junhong - CHEN, Haiyang - XING, Xinming - HOU, Xinmei - LI, Yong. *Formation mechanism of elongated beta-Si₃N₄ crystals in Fe-Si₃N₄ composite via flash combustion*. In *CERAMICS INTERNATIONAL*. ISSN 0272-8842, 2018, vol. 44, no. 8, pp. 9395-9400., Registrované v: WOS

3. [1.1] MARCHENKO, V. M. - KISELEV, V. V. *Ruby Emission in the Range 400-800 nm with Excitation by Continuous-Wave CO₂ Laser Pulses*. In *JOURNAL OF APPLIED SPECTROSCOPY*. ISSN 0021-9037, 2017, vol. 83, no. 6, pp. 1042-1045., Registrované v: WOS

4. [1.1] PARKHOMENKO, A. A. - LUKIANOVA, O. A. - KHMARA, A. N. - KRASIL'NIKOV, V. V. *Effect of the Various Oxide Additives on the Microhardness of Silicon Nitride Ceramics*. In *PROCEEDINGS OF THE 2017 IEEE 7TH INTERNATIONAL CONFERENCE NANOMATERIALS: APPLICATION & PROPERTIES (NAP)*. ISSN 2306-580X, 2017, vol., no., pp., Registrované v: WOS

ADFB Vedecké práce v ostatných domácich časopisoch – neimpaktovaných

ADFB01 PELIKÁN, P. - LIŠKA, Marek. *MO study of TD-D4H equilibrium in complexes of transition metals. II. Equilibrium in tetrafluoro and tetrabromo complexes of atoms of the first transition row*. In *Collection of Czechoslovak Chemical Communications*, 1984, vol. 49, no. 12, p. 2837-2856. ISSN 0010-0765.

Citácie:

1. [1.1] SADOK, Ines Ben Hadj - HAJLAOUI, Fadhel - BEN AYED, Hanen - ENNACEUR, Nasreddine - NASRI, Moncef - AUDEBRAND, Nathalie - BATAILLE, Thierry - ZOUARI, Nabil. *Crystal packing, high-temperature phase transition, second-order nonlinear optical and biological activities in a hybrid material: [(S)-C₇H₁₆N₂][CuBr₄]*. In *JOURNAL OF MOLECULAR STRUCTURE*. ISSN 0022-2860, 2018, vol. 1167, no., pp. 316-326., 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.

Citácie:

1. [1.1] BODNAR, Victoria - GANEEV, Alexander - GUBAL, Anna - SOLOVYEV, Nikolay - GLUMOV, Oleg - YAKOBSON, Viktor - MURIN, Igor. Pulsed glow discharge enables direct mass spectrometric measurement of fluorine in crystal materials Fluorine quantification and depth profiling in fluorine doped potassium titanyl phosphate. In SPECTROCHIMICA ACTA PART B-ATOMIC SPECTROSCOPY. ISSN 0584-8547, 2018, vol. 145, no., pp. 20-28., Registrované v: WOS

ADMA02 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.

Citácie:

1. [1.1] GOLMAKANI, M. H. - KHAKI, J. Vahdati - BABAKHANI, A. FORMATION MECHANISM OF Fe-Mo MASTER ALLOY BY ALUMINOTHERMIC REDUCTION OF $\text{MoS}_2\text{Fe}_2\text{O}_3$ IN THE PRESENCE OF LIME. In JOURNAL OF MINING AND METALLURGY SECTION B-METALLURGY. ISSN 1450-5339, 2018, vol. 54, no. 2, pp. 233-241., Registrované v: WOS

ADMA03 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. ISSN 0008-4433.

Citácie:

1. [1.1] OUZILLEAU, Philippe - GHERIBI, Aimen E. - CHARTRAND, Patrice. Prediction of CO_2/CO formation from the (primary) anode process in aluminium electrolysis using an electrothermodynamic model (for coke crystallites). In ELECTROCHIMICA ACTA. ISSN 0013-4686, 2018, vol. 259, no., pp. 916-929., Registrované v: WOS

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

ADMB01 CZÍMEROVÁ, Adriana - BUJDÁK, Juraj - GÁPLOVSKÝ, A. Reduction of the negative charge of layered silicates probed by cationic, azine dyes. In Solid State Phenomena, 2003, vol. 90-91, p. 469-474. (2003 - Current Contents). ISSN 1012-0394.

Citácie:

1. [1.1] NAKAZATO, Ryosuke - SHIMADA, Tetsuya - OHTANI, Yuta - ISHIDA, Tamao - TAKAGI, Shinsuke. Adsorption and emission enhancement behavior of 4,4'-bipyridine on dispersed montmorillonite nano-sheets under aqueous conditions. In TETRAHEDRON LETTERS. ISSN 0040-4039, 2018, vol. 59, no. 25, pp. 2459-2462., Registrované v: WOS

ADMB02 SALAMON, D. - ŠAJGALÍK, Pavol - LIŠKA, Marek. Mechanical properties and microstructure of alpha-sialon based cutting tools. In Key Engineering Materials. - Trans Tech Publications, 2005, vol. 290, p. 250-253. (2004: 0.278 - IF). (2005 - SCOPUS). ISSN 1013-9826.

Citácie:

1. [1.1] AHMED, B. A. - HAKEEM, A. S. - LAOUI, T. - AL MALKI, M. - EHSAN, M. A. - ALI, S. Low-temperature spark plasma sintering of calcium stabilized alpha sialon using nano-size aluminum nitride precursor. In INTERNATIONAL JOURNAL OF REFRACTORY METALS & HARD MATERIALS. ISSN 0263-4368, 2018, vol. 71, no., pp. 301-306., Registrované v: WOS

*AEC Vedecké práce v zahraničných recenzovaných vedeckých zborníkoch, monografiách

AEC01 DUSZA, Ján - ŠAJGALÍK, Pavol - RUDNAYOVÁ, Emöke - HVIŽDOŠ, Pavol - LENČEŠ, Zoltán. Fracture characterization of silicon nitride based layered composites. In Fracture Mechanics of Ceramics. - New York : Plenum Press, 1996, vol. 12, P. 383-398.

Citácie:

1. [1.1] TANG, Xueyuan - LI, Yongwei - CHENG, Xuan - ZHANG, Ying. In-situ formation of BN layers by nitriding boron powders in BN/ Si_3N_4 -based composite ceramics. In CERAMICS INTERNATIONAL. ISSN 0272-8842, 2018, vol. 44, no. 9, pp. 10322-10327., Registrované v: WOS

AFD Publikované príspevky na domácich vedeckých konferenciách

AFD01 LENČEŠ, Zoltán - ŠAJGALÍK, Pavol - RONCARI, E. - HIRAO, K. Design of Si_3N_4 based layered composites for multifunctional application. In Engineering Ceramics: Multifunctional Properties-New Perspectives. - Zuerich : Trans Tech Publications, 1999, p. 173-182. ISBN 0-87849-846-x.

Citácie:

1. [1.1] YU, Jun-Jie - GUO, Wei-Ming - WEI, Wan-Xin - LIN, Hua-Tay - WANG, Cheng-Yong. Fabrication and wear behaviors of graded Si_3N_4 ceramics by the combination of two-step sintering and beta- Si_3N_4 seeds. In JOURNAL OF THE EUROPEAN CERAMIC SOCIETY. ISSN 0955-2219, 2018, vol. 38, no. 10, pp. 3457-3462., Registrované v:

WOS

***AFDA Publikované príspevky na medzinárodných vedeckých konferenciách poriadaných v SR**

AFDA01 TATARKO, Peter - LOJANOVÁ, Š. - DUSZA, Ján - ŠAJGALÍK, Pavol. Fracture toughness of Si₃N₄ based ceramics with rare-earth oxide sintering additives. In Key Engineering Materials, 2009, vol. 409, p. 377-381. (2009 - SCOPUS). ISSN 1013-9826.(Fractography of Advanced Ceramics III : International Conference on Fractography of Advanced Ceramics).

Citácie:

1. [1.1] ZHONG, Jing - HUA, Guomin - CHEN, Linbo - LI, Changsheng - YANG, Jianhong - CHENG, Xiaonong. Influence of carbon on structure stability, mechanical and tribological properties of beta-Si-3(C-x,N1-x)(4) silicon carbonitride. In MATERIALS RESEARCH EXPRESS. ISSN 2053-1591, 2018, vol. 5, no. 5, pp., Registrované v: WOS

Príloha D- Údaje o pedagogickej činnosti organizácie

Semestrálne prednášky:

doc. Ing. Miroslav Boča, DrSc.

Názov semestr. predmetu: Spectroscopy

Počet hodín za semester: 28

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

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

Ing. Blanka Kubíková, PhD.

Názov semestr. predmetu: Thermodynamic of condensed systems

Počet hodín za semester: 4

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

doc. Ing. Zoltán Lenčéš, 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 Lenčéš, PhD.

Názov semestr. predmetu: Materiálová chémia

Počet hodín za semester: 4

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

doc. Ing. Zoltán Lenčéš, PhD.

Názov semestr. predmetu: Materiály pro speciální použití

Počet hodín za semester: 2

Názov katedry a vysokej školy: Vysoká škola báňská - TU Ostrava, Česká republika, Fakulta metalurgie a materiálového inženýrství

Ing. František Šimko, PhD.

Názov semestr. predmetu: Anorganická chémia 2

Počet hodín za semester: 2

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

Semestrálne cvičenia:

doc. Ing. Zoltán Lenčéš, PhD.

Názov semestr. predmetu: Materiálová chémia

Počet hodín za semester: 50

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

Ing. Jarmila Mlynáriková, PhD.

Názov semestr. predmetu: Pokročilé cvičenie z fyzikálnej chémie (1)

Počet hodín za semester: 12

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

Ing. Zuzana Netriová, PhD.

Názov semestr. predmetu: Pokročilé cvičenie z fyzikálnej chémie (1)

Počet hodín za semester: 12

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

Mgr. Patrícia Petrisková

Názov semestr. predmetu: Všeobecná a anorganická chémia

Počet hodín za semester: 40

Názov katedry a vysokej školy: Univerzita Komenského v Bratislave, Katedra anorganickej chémie

Semináre:

Mgr. Stanislav Komorovský, PhD.

Názov semestr. predmetu: Chemické výpočty (2)

Počet hodín za semester: 26

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

Terénne cvičenia:

Individuálne prednášky:

Dr. Vladimír Malkin, DrSc.

Názov semestr. predmetu: Introduction to Density Functional Theory

Počet hodín za semester: 4

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

Príloha E - Medzinárodná mobilita organizácie**(A) Vyslanie vedeckých pracovníkov do zahraničia na základe dohôd:**

Krajina	D r u h d o h o d y					
	MAD, KD, VTS		Medziústavná		Ostatné	
	Meno pracovníka	Počet dní	Meno pracovníka	Počet dní	Meno pracovníka	Počet dní
Belgicko	Anna Prnová	15				
Česko	Ondrej Hanzel	5				
	Ondrej Hanzel	3				
	Peter Tatarko	3				
	Peter Tatarko	5				
Čína	Michal Korenko	17				
Počet vyslaní spolu	6	48				

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

Krajina	D r u h d o h o d y					
	MAD, KD, VTS		Medziústavná		Ostatné	
	Meno pracovníka	Počet dní	Meno pracovníka	Počet dní	Meno pracovníka	Počet dní
Česko	Gianmarco Taveri	4				
	Jiří Hybler	7				
	Luca Bertolla	12				
Čína					Shuang Wu	181
Grécko					Eleni Gianni	93
Rakúsko					Christina Atzenhofer	27
					Igor Petrushenko	30
Ukrajina					Anna Kityk	125
Veľká Británia					Peter Cherry	275
Počet prijatí spolu	3	23			6	731

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

Krajina	Názov konferencie	Meno pracovníka	Počet dní
Belgicko	JPNM	Miroslav Boča	1
		Peter Tatarko	1
Bulharsko	MMT	Mária Chromčíková	8
Česko	IICCCL	Juraj Bujdák	3
		Michal Korenko	2
		Zoltán Lenčes	2
		František Šimko	2
	Kalorimetrický seminár	Mária Chromčíková	5
		Anna Prnová	3
	NETZSCH	Mária Chromčíková	2
		Blanka Kubíková	2
		Zuzana Netriová	2
		Anna Prnová	2
	Strategy AV21	Juraj Bujdák	3
Čína	CICC-11	Ondrej Hanzel	10
		Pavol Šajgalík	5
		Peter Tatarko	10
Francúzsko	AMARE	Patrícia Petrisková	8

	deMon Developers	Oľga Malkin	5
		Vladimír Malkin	5
	EUROCLAY	Martin Barlog	7
		Silvia Belušáková	7
		Juraj Bujdák	7
		Ľuboš Jankovič	7
		Jana Madejová	11
		Daniel Moreno	6
		Helena Pálková	7
		Eva Scholtzová	6
		Michal Slaný	9
		Peter Škorňa	7
	HT-CMC 10	Peter Tatarko	5
	MS11	Miroslav Boča	6
		Michal Korenko	6
		Blanka Kubíková	6
		František Šimko	6
Maďarsko	JTACC-V4	Mária Chromčíková	5
		Anna Prnová	5
Poľsko	ESFC	Miroslav Boča	6
Rakúsko	CESTC	Stanislav Komorovský	4
	MMQC	Oľga Malkin	6
		Vladimír Malkin	6
	UGM	Daniel Moreno	3
Singapur	ACA	Eva Scholtzová	8
Srbsko	CYSC	Hakan Ünsal	6
	SSCerM	Ondrej Hanzel	4
		Peter Tatarko	4
Španielsko	SSNMR	Anna Prnová	5
Taliansko	CEEC-TAC	Mária Chromčíková	7
	ECERS	Ondrej Hanzel	6
		Miroslav Hnatko	6
		Zoltán Lenčes	6
		Jaroslav Sedláček	6
		Pavol Šajgalík	5
		Peter Tatarko	6
		Monika Tatarková	6
		Hakan Ünsal	9
USA	ICACC	Zoltán Lenčes	6
		Pavol Šajgalík	6
Spolu	26	58	315

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

Skratky použité v tabuľke C:

ACA - 7th Annual Conference of Analytix

AMARE - International Conference of Applications of Multiscale Approaches in Environmental Chemistry

CEEC-TAC - "5th Central and Eastern European on Thermal Analysis and Calorimetry" and "14th Mediterranean Conference on Calorimetry and Thermal Analysis

CESTC - "17th Central European Symposium on Theoretical Chemistry"

CICC-11 - 11th International Conference on High-Performance Ceramics

CYSC - "13th Conference for Young Scientists in Ceramics"

deMon Developers - 19th deMon Developers Workshop

ECERS - "16th Conference and Exhibition of the European Ceramic Society"

ECERS - 16th Conference and Exhibition of the European Ceramic Society

ESFC - "19th European Symposium on Fluorine Chemistry"

EUROCLAY - "International Conference on Clay Science and Technology"
 HT-CMC 10 - "10th International Conference on High Temperature Ceramic Matrix Composites"
 ICACC - 43th International Conference and Exposition on Advanced Ceramics and Composites
 IICCCCL - Interaction of Inorganic Cluster, Cages and Containers with Light
 Interakce tavenin - "Interakce tavenin s progresivními anorganickými materiály"
 Interakce tavenin - "Interakce tavenin s progresivními anorganickými materiály"norganickými materiály"
 JPNM - EERA Joint Programme on Nuclear Materials
 JTACC-V4 - "2st Journal of Thermal Analysis and Calorimetry Conference and 7th V4 (Joint Czech-Hungarian-Polish-Slovakian) Thermal Conference
 JTACC-V4 - "2st Journal of Thermal Analysis and Calorimetry Conference and 7th V4 (Joint Czech-Hungarian-Polish-Slovakian) Thermal Conference
 Kalorimetrický seminář - 41. Mezinárodní český a slovenský kalorimetrický seminář
 KSAP-PM 2019 - "21. ročník Konference o Speciálních Anorganických Pigmentech a Práškových Materiálech"
 MMQC - XIIth Workshop: Modern Methods in Quantum Chemistry
 MMT - "21st International Conference. Materials, Methods and Technologies
 MS11 - "11th International symposium on Molten salts Chemistry and Technology"
 NETZSCH - Termická analýza NETZSCH, Alpha Technologies Brucker Optic
 SSCerM - 5th Conference of the Serbian Society for Ceramic Materials"
 SSNMR - IV School on Solid State Nuclear Magnetic Resonance and Applications
 Strategy AV21 - Strategy AV21 - Molecules and Materials for Life
 UGM - "Materials Design User Group Meeting"

Príloha F - Vedecko-popularizačná činnosť pracovníkov organizácie SAV

Meno	Spoluautori	Typ ¹	Názov	Miesto zverejnenia	Dátum alebo počet za rok
Juraj Bujdák		RO	Nočná pyramída - hosť	SRo 1	30.4.2019
Viliam Pavlík		EX	Nájdí v sebe vedca	ÚACH	29.5.2019
Anna Prnová	J. Valúchová, R. Klement, D. Galusek	PB	Študentská vedecká konferencia Nová Dubnica	Nová Dubnica	1.4.2019
		EX	Exkurzia pre študentov denného štúdia programu Anorganická technológia FCHPT STU	ÚACH SAV	4.4.2019
Peter Tatarko		PB	Nové trendy vo vývoji pokročilej keramiky na ÚACH SAV	FCHPT STU	11.12.2019
		PB	Skúsenosti držiteľa grantu H2020-IF-MSCA	CVTI	23.5.2019
Miroslav Boča		PB	Prvky známe aj neznáme	ChemZi	1
Ing. Dušan Galusek		TL	Anketa SME	SME veda a technika	5
Viliam Pavlík		PB	Letná škola mladých vedcov 15.-19. 7. 2019	ÚACH	1

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