

11th Workshop of Slovak Clay Group

**CLAY MINERALS AND SELECTED
INDUSTRIAL MINERALS IN MATERIAL
SCIENCE, APPLICATIONS,
AND ENVIRONMENTAL TECHNOLOGY**

Book of Abstracts

JUNE 2 – 4, 2025, Červený Kláštor, SLOVAKIA

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ORAL PRESENTATIONS

A COMPARATIVE ANALYSIS OF POLY (2-METHYL-2-OXAZOLINE)-MODIFIED MONTMORILLONITE VS SAPONITE FOR STYRENE ADSORPTION BY DFT-D3 STUDY

A. Asbat^{1*}, E. Scholtzová¹

¹ Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

* e-mail:ayesha.asbat@savba.sk

KEYWORDS: Smectites | Clay-polymer hybrids | Styrene | DFT

The development of efficient adsorbents to remove chemical pollutants has garnered significant attention due to growing environmental concerns. This study investigates the potential of clay-polymer hybrid materials for the adsorption of styrene, a hazardous environmental pollutant [1]. Because of the natural abundance of clays, their affordability, high cation exchange capacity, and environmental sustainability, the materials are intriguing choices for handling common chemical pollutants. The functionality of the resulting clay-based composites was enhanced, however, when Poly(2-methyl-2-oxazoline) - PMOx was added to the structures of smectites, such as saponite (Sap) and montmorillonite (Mt), using surface modification [2].

To accomplish this, we used Density Functional Theory (DFT) with D3 scheme for corrections of dispersion forces (DFT-D3) to investigate the adsorption potential of Mt+PMOx and Sap+PMOx composites [3]. Our findings demonstrated that Sap+PMOx composite outperformed Mt+PMOx composite in terms of styrene adsorption capabilities.

These findings demonstrated, Sap+PMOx was more effective for immobilisation of styrene, making it a potentially useful substance for environmental cleanup. This work contributes to our understanding of the durability and interactions of clay-polymer hybrids, which may result in more environmentally friendly methods of eliminating industrial pollutants.

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COMPARISON OF ADSORPTION OF PERFLUOROBUTYRIC ACID AND PERFLUOROHEXANOIC ACID ON MONTMORILLONITE CLAY USING DFT-D3 METHOD

S. Bashir^{1*}, E. Scholtzová¹

¹ Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

*sanam.bashir@savba.sk

KEYWORDS: Perfluoroalkyl acids | Montmorillonite | DFT-D3 | Adsorption

Perfluoroalkyl acids (PFAAs) represent a broad category of chemicals noted for their robust carbon-fluorine bonds, which provide remarkable stability, resistance to degradation in the environment, and specialized surfactant functions. These substances have been widely utilized in numerous industrial and consumer products, including fire-fighting foams, lubricants, and coatings that repel water or stains for textiles, paper, and leather. Due to their extensive use and lasting presence in the environment, PFAAs have been found globally in water, soil, sediments, air, and biological tissues, even in isolated areas distant from industrial activities. Their pervasive presence in the environment, along with their tendency to bioaccumulate and the potential negative impacts on both wildlife and human health, has sparked considerable concern. Understanding the sorption mechanisms of PFAAs to clay minerals is critical because minerals are major constituents of natural sediments and soils, playing a key role in the mobility, bioavailability, and fate of pollutants in aquatic and terrestrial environments. Sorption processes can significantly impact the transport behavior of PFAAs, affecting their partitioning between the aqueous phase and solid phases in the environment [1].

This study investigates the sorption behaviors of two PFAAs with different chain lengths on montmorillonite (Mt) with the goal to analyze of adsorption energies and evaluating the stability of the resulting systems. The Density Functional Theory (DFT) method implemented in the Vienna *ab Initio* Simulation Package (VASP) [2] is employed to explore the interactions within the proposed models. Structural optimizations are performed using the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional to account for exchange-correlation effects. A comparative analysis is conducted for Mt with perfluorobutanoic acid (Mt–PFBA), and perfluorohexanoic acid (Mt–PFHA).

The findings confirmed the stability of hybrid systems of Mt clay with PFBA and PFHA and highlighted differences in structural stability attributed to variations in chain length. These results reinforce the potential of using natural clays as efficient adsorbents for the removal of PFAAs from contaminated water sources.

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NOVEL FUNCTIONAL GEOPOLYMER COMPOSITES BASED ON CALCINED CLAYS WITH EXCELLENT IMMOBILIZATION PROPERTIES

A. Bershadskiy^{1*}, A. Juriček¹, Š.J. Rezbárik², L. Vavrinčová², M. Horník², M. Slaný^{1,3}

¹ Department of Materials Engineering and Physics, Faculty of Civil Engineering, Slovak University of Technology, Radlinského 11, 810 05, Bratislava, Slovakia

² Institute of Chemistry and Environmental Sciences, Faculty of Natural Sciences, University of Ss. Cyril and Methodius in Trnava, Nám. J. Herdu 2, 917 01, Trnava, Slovakia

³ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

* anton.bershadskiy@stuba.sk

KEYWORDS: Geopolymer composites | Metabentonite | Metakaolin | Immobilization

Geopolymer composites (GPs) derived from metabentonite (MB) and metakaolin (MK) were prepared by calcination at 700 and 800 °C, followed by alkali activation with 10 and 20 wt.% NaOH solutions. Their structural and morphological characteristics were analyzed using FTIR, PXRD, and SEM. The retention and distribution of artificial radionuclides ⁶⁰Co and ¹³⁷Cs in the GPs and leachate were quantified by scintillation gamma spectrometry.

PXRD and FTIR analyses showed that in MK-based GPs, zeolitic phases increased with higher alkaline activator concentrations, with zeolite A and P being dominant. In MB-based GPs, faujasite and gobbinsite were predominant at higher NaOH concentrations. SEM confirmed the formation of cuboidal crystalline structures and geopolymeric gel in both systems.

All synthesized GPs, with a weight ratio of geopolymers to solution ranging from 1:1,000 to 1:10,000, demonstrated significant binding efficiencies for Co and Cs, reaching approximately 90 % of the total Co and Cs present in solutions containing 100 μmol/dm³ of both radionuclides. To gain deeper insights into the adsorption behavior of ¹³⁷Cs, a geopolymer composite sample calcined at 800 °C and activated with 10 wt.% NaOH (GP10_MB800) was selected for further investigation. It was found that Cs adsorption efficiency increased linearly with the amount of GP (0.5 to 4.0 g/dm³) in a 1,000 mg/dm³ CsCl solution containing ¹³⁷CsCl. However, the specific adsorption of Cs (mg/g) decreased exponentially. Cs adsorption kinetics showed rapid metal ion binding until equilibrium was reached, with $[Cs]_{\text{adsorbent}} : [Cs]_{\text{solution}}$ ratio stabilizing. Cs adsorption efficiency decreased linearly with higher Cs concentrations, while specific adsorption increased nonlinearly, indicating gradual saturation of GP. Adsorption isotherms fit better with the Langmuir model ($R^2 = 0.973$) than the Freundlich model ($R^2 = 0.960$), predicting a maximum adsorption capacity of $Q_{\text{max}} = 116 \pm 10$ mg/g for GP10_MB800.

These results suggest that geopolymer composites based on metabentonite (MB) and metakaolin (MK) are effective for remediating environments contaminated by artificial radionuclides. Their ability to adsorb and retain radionuclides like ⁶⁰Co and ¹³⁷Cs makes them a promising option for environmental remediation.

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PHOTOACTIVE NANOCOMPOSITES BASED ON SAPONITE: A PROMISING STRATEGY FOR MRSA BIOFILM ERADICATION

K. Bilská^{1*}, M. Pribus³, J. Bujdák^{2,3}, H. Bujdáková¹

¹ Department of Microbiology and Virology, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15, Bratislava, Slovakia

² Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15, Bratislava, Slovakia

³ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36 Bratislava, Slovakia

* bilaska6@uniba.sk

KEYWORDS: Nanocomposite | Anti-Biofilm | Photoactive | *Staphylococcus*

Methicillin-resistant *Staphylococcus aureus* (MRSA) strains can form biofilms on a wide range of surfaces and often exhibit resistance to multiple antibiotics, complicating treatment. This research evaluates photoactive nanocomposites (NC) with antibiofilm properties and investigates their primary mechanism of action and bacterial responses to the oxidative stress.

Polyurethane (PU) modified with a saponite (Sap) and poly(diallyldimethylammonium) (PDDA; 1.5 mmol/g) layer functionalized with phloxine B (PhB) was used. PhB concentrations varied from 0.0 to approximately 0.45 mmol·g⁻¹. Standard strain *S. aureus* CCM3953 (CCM) and clinical isolates *S. aureus* S61 and L12 were used. The effectiveness of NC was tested on 24-h biofilms before and after irradiation with a green laser (IR; $\lambda = 532$ nm, 100 mW, duration 120 s). Reactive oxygen species (ROS) production was evaluated using the ROS-GloTM H₂O₂ assay, and oxidative stress-related gene expression (*sodA*, *kata* and *ahpC*) was assessed by RT-qPCR with expression calculated by the 2^{ΔΔC_T} method.

The highest antibiofilm effectiveness was observed on NC modified with the maximum concentration of PhB after irradiation, showing a 2.8-, 2.39- and 2.64-log reductions for CCM, S61 and L12, respectively after irradiation. The results demonstrated that the effectiveness of the NC was dependent on the PhB concentration. A significantly increased amount of H₂O₂ was detected after irradiation compared to the NC before irradiation for each tested strain. ROS production showed more than 15-, 17-, and 10-fold increases in relative luminescence units (RLU) for CCM, S61, and L12, respectively. The mechanism of action was confirmed by increased expression of the *sodA* and *kata* genes and decreased expression of the *ahpC* gene in the tested strains.

These findings highlight the potential of photoactive NC functionalized with PhB as an effective strategy against MRSA biofilms. The observed induction of oxidative stress-related responses suggests a promising mechanism for overcoming bacterial resistance.

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SMECTITES AS A PLATFORM FOR TUNING THE PHOTOPHYSICAL PROPERTIES OF ORGANIC DYES

P. Boháč^{1*}, V. Planetová¹, J. Bujdák^{1,2}

¹ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

² Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, Bratislava, 841 04, Slovakia

* peter.bohac@savba.sk

KEYWORDS: Smectite-based hybrid materials | Molecular aggregation | Surface-fixation induced emission

This work highlights recent advances in understanding how layered silicates—particularly smectites serve as functional platforms for controlling the photophysical behavior of organic dyes. Smectites, due to their layered charge distribution, swellable interlayer space, and high specific surface area, offer unique opportunities to modulate dye properties through adsorption and intercalation.

The most frequently observed phenomena in such hybrid systems are molecular aggregation; along with related effects such as metachromasy, aggregation-induced quenching, and even aggregation-induced emission; and surface-fixation induced emission (SFIE). In the latter, the prevention of rotational and vibrational motions through surface fixation suppresses non-radiative deactivation pathways, thereby favoring visible emission.

Importantly, smectites in these systems do not act merely as passive carriers. By selecting appropriate smectite characteristics and tuning reaction conditions, it is possible to actively control the final properties of the resulting hybrid materials. This work presents an overview of the role of smectites and their properties in photoactive hybrid systems.

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FROM DNA TO CLAY: PROBING LIGHT-UP PHENOMENA

J. Bujdák^{1*,2}

¹ Department of Physical and Theoretical Chemistry, Comenius University in Bratislava, Faculty of Natural Sciences, Ilkovičova 6, 842 15, Bratislava, Slovakia

² Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

* juraj.bujdak@uniba.sk

KEYWORDS: Luminescence | Organic dyes | Layered silicates | Adsorption

The light-up effect has been studied primarily in connection with the detection of nucleic acids, using molecular probes that exhibit weak fluorescence in solution but emit strongly after binding to DNA or RNA. A similar phenomenon was observed in clay mineral systems, where dyes exhibit strong emission upon adsorption or intercalation in silicate layers. While the light-up effect in nucleic acid systems is used for analytical purposes, its manifestation in hybrid clay-dye hybrids opens up new possibilities for the development of photoactive materials.

The light-up phenomenon forms the basis for some of our ongoing research projects. This presentation will explore conceptual parallels between the effects in the systems based on nucleic acid and clay minerals. Understanding the details of both systems may provide a deeper insight into the underlying mechanisms, which is essential for identifying the key direction of the research. Key factors influencing fluorescence, such as surface interactions, restricted molecular mobility, local polarity, and molecular aggregation, will be critically investigated.



Particular attention should be paid to exploring molecular structures of luminophores, which exhibit strong light-up behavior. The influence of clay parameters such as particle size and charge, hydration state, and chemical modification are also important. The presentation will address the challenges associated with photophysical methods developed for nucleic acids. Mineral

substrates with tunable properties provide a cost-effective and robust platform for studying the properties of various molecular probes. The interdisciplinary approach can lead to innovative applications in photochemistry, environmental sensing, and science education. Ultimately, this work bridges the gap between bioanalytical chemistry and materials science and opens new avenues for the practical use of readily available or newly synthesized luminophores.

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FABRICATION OF NANOCOMPOSITE HYDROGELS FEATURING FUNCTIONAL PHOTOACTIVE SURFACES FOR PHOTODYNAMIC INACTIVATION

V. George¹, P. Boháč¹, J. Bujdák^{1,2}

¹ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

² Department of Physical and Theoretical Chemistry, Comenius University in Bratislava, Faculty of Natural Sciences, Ilkovičova 6, 842 15, Bratislava, Slovakia

* vinny.george@savba.sk

KEYWORDS: PDI | Hydrogel nanocomposite | Clay mineral | Photosensitizer

Photodynamic inactivation (PDI) is a promising antibiotic-free antimicrobial strategy promoting wound healing. Its efficacy relies on the controlled generation of reactive oxygen species (ROS) by photosensitizers (PSs). Hydrogels have been widely employed as PS carriers for PDI. However, limitations such as low light transmission, uncontrolled PS and ROS release, and poor solubility, stability, and bioactivity of many PSs under physiological conditions persist [1]. Additionally, achieving uniform PS dispersion within hydrogels remains challenging.

As low-cost, eco-friendly inorganic hosts for dyes, smectites sometimes offer enhanced fluorescence, photoactivity, and stability while reducing photodegradation of adsorbed dye molecules [2]. In this study, organoclays of synthetic saponite (Sap) were used to load the PS phloxine B (PhB). Thin films of PhB-intercalated organoclays, only a few μm thick, were prepared via vacuum filtration. A hydrogel precursor consisting of poly(vinyl alcohol) (PVA) and glycerol was cast onto these films, allowing partial penetration into the organoclay layer and *in situ* cross-linking to form the hydrogel. In this method, a thin nanocomposite layer was formed on the hydrogel surface due to the penetration of the precursor during the crosslinking [3], [4].

Unlike bulk loading, this strategy allows better control over the PS content by concentrating the active molecules at the surface while preserving the hydrogel bulk unchanged. Absorption and fluorescence spectroscopy revealed that increasing PhB loading caused fluorescence quenching due to dye aggregation. X-ray diffraction (XRD) confirmed the structural changes due to PhB intercalation, while Fourier-transform infrared (FTIR) spectroscopy suggested hydrogen bonding as the dominant interaction mechanism.

This novel fabrication approach offers precise control over PS distribution, enhancing hydrogel-based PDI systems' therapeutic potential and clinical applicability.

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MECHANICAL AND STRUCTURAL PROPERTIES OF CEMENT CONCRETES ON RECYCLED AGGREGATES

A. Chystiakov^{1*}, I. Medved², M. Slaný^{1,3}

¹ Department of Materials Engineering and Physics, Faculty of Civil Engineering, Slovak University of Technology in Bratislava, Radlinskeho 2766/11, 810 05, Bratislava, Slovakia

² Department of Materials Engineering and Chemistry, Faculty of Civil Engineering, Czech Technical University in Prague, Thákurova 7, 166 29, Prague, Czech Republic

³ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

* artem.chystiakov@stuba.sk

KEYWORDS: Concrete | Recycled aggregates | Rigid pavement | Road construction

The study investigates the development of concrete mixtures using various natural and recycled aggregates, specifically river gravel, quartz sand, coarse and fine fractions of recycled concrete aggregate, and coarse and fine fractions of recycled masonry aggregate. The concretes were formulated with two distinct cement contents: 300 and 350 kg/m³ of concrete mixture, aiming to explore the potential for use in the construction of lower layers of rigid pavements. For this purpose, mixtures with minimal workability (S1) were designed to maximize mechanical strength.

The mechanical and structural properties of concretes based on natural and recycled aggregates of different types and fraction were studied experimentally. Namely, the prototypes were tested for density, water absorption, frost resistance, compressive and flexural tensile strengths, and impact resistance. For physicochemical characterization FTIR, TGA/DSC and SEM analysis were performed.

The experimental results demonstrate that the concretes exhibit relatively high flexural tensile strength (2.82 – 3.84 MPa) and frost resistance (F100), which are critical characteristics for materials used in road pavement applications. The concretes also exhibit substantial compressive strength (27.1 – 53.4 MPa) and impact resistance (1.90 – 2.49 J/cm²). Structural analysis further confirms the absence of deleterious inclusions that could promote corrosion or pose risks to human health. FTIR analysis supports the adequacy of the sample preparation and reveals the presence of a carboxylate-based additive, which enhances the workability of the mixtures. TGA/DSC analysis indicates the decomposition of water, calcium hydroxide, and calcium carbonates, while SEM observations confirmed the presence of C-S-H phases and ettringite.

The developed concretes meet regulatory requirements for lower layers of rigid pavements. Thus, using secondary coarse and fine aggregates in pavement concretes offers a viable solution from both construction and environmental sustainability perspectives, due to the use of recycled materials.

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EXPLORING THE ADSORPTION PROPERTIES OF BODIPY ON SAPONITE FOR FUNCTIONAL HYBRID MATERIALS

L. K. Santos¹, P. Boháč¹, J. Bujdák^{1,2}

¹ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

² Department of Physical and Theoretical Chemistry, Comenius University in Bratislava, Faculty of Natural Sciences, Ilkovičova 6, 842 15, Bratislava, Slovakia

* leonardo.kleman@savba.sk

KEYWORDS: BODIPY | Synthesis | Saponite | Hybrid Materials

Boron-dipyrromethene (BODIPY) dyes are renowned for their photostability, tunable fluorescence, and structural adaptability, making them ideal building blocks for hybrid materials. [1, 2] In this study, a series of thirteen BODIPY derivatives was synthesized and characterized, featuring both cationic and neutral structures with different polarity, to investigate their interactions with saponite (Sap), a layered silicate with a negatively charged surface and growing relevance in materials science.

The structural and photophysical properties of the dyes were investigated using ¹H, ¹³C, and ¹⁹F NMR, UV-Vis absorption, FTIR, and fluorescence spectroscopy. Of the synthesized compounds, two representative dyes, one cationic and one neutral, were selected for in-depth studies with Sap to explore how molecular charge and polarity affect the binding behavior and fluorescence response. Depending on the compound, both fluorescence quenching and surface-induced emission were observed. The results reveal distinct interaction mechanisms and open up new possibilities for BODIPY-based hybrid materials in applications such as sensing, catalysis, and optoelectronics.

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FTIR SPECTROSCOPIC STUDY OF MODIFIED CLAY MINERALS AS COMPONENTS IN FUNCTIONAL MATERIALS DESIGN

P. Labib Shotorban^{1*}, H. Pálková¹

¹ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

*parisa.labib@savba.sk

KEYWORDS: FTIR spectroscopy | Clay minerals | Acid-treatment | Chitosan

The modification of clay minerals with organic materials has attracted significant interest due to their potential in a wide range of applications. In this study, smectites were treated with acetic and citric acids and subsequently combined with biopolymer chitosan (CTS) to prepare nanocomposite materials. The structural evolution of the clay minerals during each stage of modification was characterized by Fourier-transform infrared (FTIR) spectroscopy in both the middle and near infrared (MIR and NIR) regions.

Four smectites, dioctahedral montmorillonite Kopernica (Slovakia) and trioctahedral hectorites natural (SHCa, USA) and synthetic (SWN Sumecton, Kunimine Industries, Japan), and Laponite RD (Rockwood Additives, United Kingdom) hectorites were studied. Upon treatment with organic acids, MIR spectra of the montmorillonite exhibited no significant changes in the absorption bands attributed to O–H and Si–O groups. Whereas, the hectorites showed reduced absorption intensities at 3680 and 670 cm⁻¹, referring to partial decomposition of layers and removal of central atoms. Also, new bands appeared at 1074 cm⁻¹ and 800 cm⁻¹, which were identified as amorphous silica. Their relative intensity followed the order SHCa ≈ SWN < Laponite, reflecting clay-specific reactivity under acidic conditions. In the NIR spectra, overtone (2ν) and combination (ν+δ) bands associated with Si–OH groups were observed near 7320 and 4420 cm⁻¹, respectively, in the hectorites, providing further evidence for acid-induced structure alteration.

Following chitosan incorporation, the SWN–CTS sample showed new spectral features characteristic of the biopolymer, including broad absorption bands at 3200–2800 cm⁻¹ (N–H and C–H stretching) and sharper bands at 1431 and 1601 cm⁻¹ assigned to C–N and C=O stretching [1]. However, amorphous silica-related bands remained detectable, with reduced intensity even upon incorporation of chitosan. The intensity of the bands of amorphous silica, particularly near 800 cm⁻¹ was lower compared to smectites treated only with organic acids. This observation confirms a decrease in layer decomposition within the nanocomposite samples.

These initial results confirm that FTIR spectroscopy effectively reveals even subtle changes in clay-biopolymer systems, emphasizing the role of acidic treatment and polycation incorporation in tuning the characteristics of smectite-based nanocomposites.

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MOLECULAR RECOGNITION MATERIALS: FROM SOLUTION HOST-GUEST CHEMISTRY TO SUPRAMOLECULAR MATERIALS

J. Labuta^{1,2*}

¹ Institute of Organic Chemistry and Biochemistry (IOCB), Fleming sq. 2, 160 00, Prague, Czech Republic

² National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

* Labuta.Jan@nims.go.jp

KEYWORDS: Porphyrin | Layered double hydroxide | Sensing | Actuation

Porphyrins are functional dyes that play an essential role in living organisms. Using synthetic modifications of the porphyrin macrocycle, we have demonstrated various properties and applications of these derivatives, such as trace water impurity detection [1], chirality detection (Fig.1a) [2], pH or selective anion sensing, etc. This molecular sensing is based on supramolecular concepts, however, it is still limited to the solution state. Hybrid materials combining these concepts with powdery materials, such as layered double hydroxides (LDH), exhibit even more practical applications.

We employed modified porphyrins adsorbed at the surface of LDH particles for naked-eye colorimetric detection of methanol from ethanol [3]. We also show that carbonate anion intercalated in LDH undergoes a rapid exchange with atmospheric CO₂ under ambient conditions, which implies that the global carbon cycle involving exchange between lithosphere and atmosphere CO₂ is much more dynamic than previously thought (Fig.1b) [4]. We also made hybrid materials composed of a powdery mixture of nitrite (NO₂⁻)-type layered double hydroxide (LDH) and ascorbic acid loaded on silica gel (AASiO₂) for steady generation of therapeutic doses of NO gas (5-20 ppm at 0.5 L/min for 24 h), which can be used for medical applications, such as treatment of viral pneumonia, bronchitis, acute respiratory distress syndrome, etc [5].

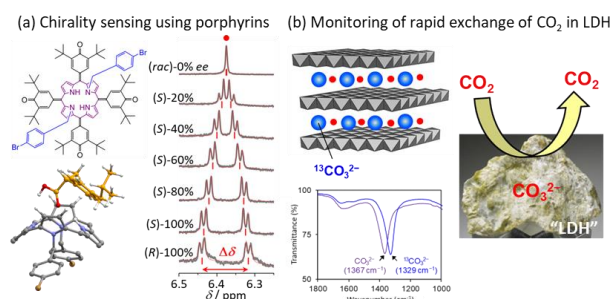


Figure 1. (a) Chirality (i.e., enantiomeric excess detection) using NMR and symmetrical porphyrin-type molecule. (b) IR study of the exchange rate of atmospheric CO₂ and CO₂ embedded in LDH.

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TECHNO-MINERALOGICAL ANALYSIS OF HATVAN CULTURE CERAMICS FROM VČELINCE, SOUTH-CENTRAL SLOVAKIA

D. Pinzón^{1*}, K. Šarinová¹, P. Uhlík¹, D. Oravniková²

¹ Department of Mineralogy, Petrology and Economical Geology, Faculty of Natural Sciences, Comenius University of Bratislava, Ilkovičova 3278/6, 841 04, Bratislava, Slovakia.

² Institute of Archaeology, Slovak Academy of Sciences. Akademická 2, 949 21, Nitra, Slovakia.

* pinzon1@uniba.sk

KEYWORDS: Ceramic technology | Raw material provenance | Hatvan culture | Exchange networks

The Bronze Age site of Včelince, located in the Rimavská kotlina basin of central-southern Slovakia, preserves a stratified archaeological sequence comprising seven soil layers. These strata contain evidence of five successive cultural phases: the Hatvan, Hatvan-Otomani, Koszider, Piliny, and Kyjatice cultures [1]. This study presents the first technological and mineralogical analysis of ceramics from layers VI and VII, attributed to the Hatvan culture and radiocarbon dated to 3710 ± 38 BP [2]. The aim is to investigate early Bronze Age ceramic production and raw material sourcing in the region.

A multi-method approach—macroscopic and microscopic analysis, SEM-EDS, and EPMA-WDS—was applied to assess inclusion types, clay matrix texture, elemental composition, and firing conditions. Fine ceramics were mostly reduced-fired with low porosity, while coarse types were more heterogeneously fired, with higher porosity and frequent microfractures, consistent with regional patterns [3].

Three compositional groups were identified. The most common includes granitoid, sandstone/siltstone, and gneiss, aligning with local geology [4]. A second group contains sedimentary inclusions with biogenic silica (sponge spicules) and calcite (VC_014), suggesting use of Paleogene or Neogene sediments and possible post-depositional alteration [5]. A third group with rhyolitic tuff and pumice suggests non-local origins and long-distance exchange.

The results indicate both local ceramic production and broader exchange networks. Variations in raw material and technique reflect dynamic interactions and evolving practices in early Bronze Age society. This study provides a baseline for future work on later site phases.

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INSIGHTS INTO THE PHOTOPHYSICAL PROPERTIES OF DYE/LAYER SILICATE HYBRID SYSTEMS

V. Planetová^{1*}, P. Boháč¹, J. Bujdák², P. Hrobárik³

- ¹ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia
- ² Department of Physical and Theoretical Chemistry, Comenius University in Bratislava, Faculty of Natural Sciences, Ilkovičova 6, 842 15, Bratislava, Slovakia
- ³ Department of Inorganic Chemistry, Comenius University in Bratislava, Faculty of Natural Sciences, Ilkovičova 6, 842 15, Bratislava, Slovakia

* viktoria.planetova@savba.sk

KEYWORDS: Hemicyanine Derivatives | Layered Silicates | Photophysical Properties | Surface-Fixation Induced Emission

By combining layered silicates with organic dyes, a hybrid photofunctional material can be obtained. The enhancement of luminescence in these systems is primarily attributed to the immobilization of dye molecules on the two-dimensional surface of the silicate, with the phenomenon of Surface-Fixation Induced Emission (S-FIE) playing a key role. Suppression of mobility reduces quenching via rotational movements and other adverse relaxation pathways [1]. These materials hold significant potential for next-generation applications in optoelectronics, bioimaging, and photomedicine [2].

In this study, we prepared hybrid dispersions by combining cationic benzothiazole derivatives with synthetic saponite (Sap). Sap is a layered silicate from the smectite group, which was selected for its low surface charge and small particle size. These properties have proven to be ideal for the preparation of S-FIE-based materials [3]. Five benzothiazole derivatives with varying triarylamine subunit rigidity were investigated to assess their impact on S-FIE and overall photophysical behaviour. The dispersions were prepared at different dye/Sap ratios and characterized via spectroscopic techniques.

Our results indicate that luminescence enhancement depends on both the dye structure and the dispersion composition. The highest quantum yields (~10%) were observed for dyes with freely rotatable triarylamine and carbazole substituents, whereas planar derivatives formed aggregates, resulting in fluorescence quenching. Additionally, we developed a model based on energy transfer and molecular distances at the surface to explain fluorescence trends in S-FIE systems.

This study advances the understanding of structure-property relationships, providing insights for optimizing future photofunctional materials.

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ADSORPTION PROPERTIES OF POLY-(N-BUTYLETHYLENEIMINE)-MODIFIED MONTMORILLONITE IN REMOVAL OF Cr(VI) FROM WATER SOURCES - COMPUTATIONAL AND EXPERIMENTAL STUDIES

P. Škorňa^{1*}, L. Jankovič³, E. Scholtzová¹, D. Tunega²

¹ Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, 845 36, Bratislava, Slovakia

² Institute for Soil Research, University of Natural Resources and Life Sciences, Peter-Jordan-Strasse 82, A-1190, Wien, Austria

³ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

* peter.skorna@savba.sk

KEYWORDS: Polymeric surfactant | DFT-D3 | Montmorillonite | Adsorption

Adsorption is a popular and highly efficient method for removing heavy metal pollutants, including Cr(VI), from water sources. It involves using an adsorbent material to bind heavy metal ions to its surface, thereby removing contaminants from the water. Common adsorbents used for this purpose include activated carbon [1], clays [2], zeolites [3], and various modified materials [4]. Poly-(N-butyl ethyleneimine) polymer matrices, used as modifiers of clay minerals, belong to the group of branched cationic PEI polymers, which contain alternating hydrophobic groups (–CH₂–CH₂–) and hydrophilic units (NH–) in their macromolecular chains. Moreover, they can be easily protonated in an acidic solution to electrostatically adsorb contaminants with a negative charge.

This work presents the combined computational DFT-D3 and experimental studies of the adsorption properties of poly-(N-butyl ethyleneimine)-modified montmorillonite in the removal of hazardous pollutants, Cr(VI), in this case. The main aim of this investigation is to provide a comprehensive structural study, including the calculation of structural stability and the determination of the strength and number of hydrogen interactions of the studied system. Moreover, the calculated vibrational modes using ab initio molecular dynamics were analysed in detail and compared with measured FTIR spectra. The calculated projected vibrational density of states was used to identify the individual vibrational modes and overlapped bands in the measured FTIR spectra.

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POSTER PRESENTATIONS

LABORATORY TECHNOLOGICAL RESEARCH OF QUARTZITES FROM LOCALITY ŽIRANY

A. Bekényiová^{1*}, Z. Danková¹, Z. Kollová¹, E. Fedorová¹, P. Bačo¹, J. Briančin²

¹ State Geological Institute of Dionýz Štúr, Regional centre Košice, Jesenského 8, 040 01, Košice, Slovak Republic

² Institute of Geotechnics, Slovak Academy of Sciences, Watsonova 45, 040 01, Košice, Slovak Republic

* alexandra.bekenyiova@geology.sk

KEYWORDS: Quartzite | Treatment | Silicon metal

The basic raw materials for the production of high-purity silicon are silicon raw materials. The Slovak Republic has suitable mineral resources on its territory. Some parts of deposits of windblown sands and quartzites represent also one of the possible sources of input raw materials for the production of high-purity silicon. [1].

Silicon metal was added to the list of critical minerals for European Union countries in 2014 [2]. Silicon metal has started a revolution in the electronics industry in the production of semiconductors and electronic components. The world's main producers of Si metal are China (66%), the United States (8%), Norway (6%) and France (4%) [3].

The principles for the production of ferrosilicon (FeSi) and metallurgical grade silicon (MG-Si) are similar, and both involve the reduction of quartzes (or quartzites) with carbon in a submerged arc furnace (SAF) at high temperatures [4].

Quartzites from locality Žirany (Slovakia) were selected as input raw materials for technological research. On the basis of input analyses, laboratory technological processing of raw materials were suggested and realized with the aim of obtaining suitable intermediate products for the silicon metal production. In order to achieve higher purity in the quartzite samples from locality Žirany, it is necessary to use more process nodes. The most effective treatment method appears to be the separation of the fraction below 0.1 mm and subsequent chemical leaching of the raw material of grain size above 0.1 mm in HCl.

The above treatment of quartzites allows their better recovery than just use for construction purposes, e.g. for the production of ferrosilicon, which can then also be used in the silicothermal method for the production of metallic magnesium.

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OXYANION REMOVAL BY CARBONATE-BASED LAYERED DOUBLE HYDROXIDES: RELATED MECHANISMS AND STRUCTURAL CHANGE INVESTIGATIONS

B. Böserle Hudcová^{1*}

¹ Department of Environmental Geosciences, Faculty of Environmental Sciences, Czech University of Life Sciences Prague, Kamýcká 129, 165 00, Praha-Suchdol, Czech Republic

* hudcovab@fzp.czu.cz

KEYWORDS: Layered double hydroxides | Oxyanion | Adsorption | Stability

The mobility of elements in the environment is significantly influenced by mineral-water interfaces, including various types of clays. Among these, layered double hydroxides (LDHs), i.e., anionic clays, have attracted considerable attention due to their high adsorption performance toward oxyanions, making them promising materials for environmental remediation. Numerous studies have examined the adsorption capabilities of LDHs, with some combining mechanistic modeling and solid-phase analyses to provide direct insights into removal mechanisms [1-4]. However, the practical use of LDHs also requires cost-effective solutions, achievable by replacing pure chemicals with waste-derived materials, either as structural matrices (e.g., pyrolyzed waste) or alternative metal sources for LDH synthesis (e.g., Fe sludge) [5-6]. This contribution summarizes findings on the role of carbonate-based Mg-Fe LDHs in capturing oxyanions, including related mechanisms and structural changes, and outlines more economical LDH-based alternatives. Combinations of solid-state analyses (e.g., XRD, FTIR, XPS) are particularly valuable for investigating adsorption mechanisms on the LDH surface. At low oxyanion concentrations, surface complexation dominates. However, at higher concentrations, additional processes such as surface precipitation occur, and in some cases, LDH structures gradually degrade. To improve LDH stability and reduce costs, composite materials using pyrolyzed waste and/or alternative metal sources were synthesized and tested. These materials also demonstrated noticeable removal efficiency towards oxyanions and sufficient stability, indicating a potential pathway for LDH applications in real environmental engineering systems.

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GLOBAL OPTIMIZATION OF CHEMICAL CLUSTER STRUCTURES VIA GENETIC ALGORITHM

Š. Budzák^{1*}, M. Mojžiš², B. Michalíková²

¹. Department of Chemistry, Matej Bel University, Tajovského 40, 97404, Banská Bystrica, Slovakia

². Department of Computer Science, Matej Bel University, Tajovského 40, 97404, Banská Bystrica, Slovakia

* Simon.Budzak@umb.sk

KEYWORDS: Genetic Algorithm | Global Optimization | Theoretical Calculation | Aggregation

This work presents a computational approach for determining the global energy minimum structures of chemical clusters using genetic algorithms. The foundational principles of optimization problems and genetic algorithms are introduced, followed by a detailed exploration of chemical cluster optimization and relevant computational models. The central outcome of this research is the development and implementation of a program, GenCluster, which employs a genetic algorithm to efficiently search for the lowest energy configurations of molecular aggregates. The design and implementation of this algorithm are thoroughly described. Validation of GenCluster's performance is presented through a comparative study on small gold clusters and water molecules, demonstrating its reliability and significant speed advantage over more systematic methods, albeit with a trade-off in exhaustiveness [1]. Finally, we present the successful application of this methodology to the aggregation of R123 dye.

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PHOTODYNAMIC INACTIVATION OF STAPHYLOCOCCUS AUREUS USING ERYTHROSIN B: AN ANTIBIOFILM APPROACH

L. Bugyna^{1*}, K. Bilská¹, P. Boháč³, M. Pribus³, J. Bujdák^{2,3}, H. Bujdáková¹

¹ Department of Microbiology and Virology, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15, Bratislava, Slovakia

² Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15, Bratislava, Slovakia

³ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

* larysa.bugyna@uniba.sk

KEYWORDS: *S. aureus* | Erythrosin B | Nanocomposite | Photodynamic inactivation

Erythrosine B (EryB), a red xanthene dye, has gained attention as a potential photosensitizer to inhibit Gram-positive bacteria such as *Staphylococcus aureus* and their biofilms. This study addresses the photoactive properties of EryB and evaluates the efficacy of polyurethane (PU)-based antimicrobial materials with a layer of saponite (SAP) modified with poly(diallyldimethylammonium) cations (PDDAC) and functionalized with EryB [1].

All experiments were performed with the standard strain *S. aureus* CCM 3953 in the Mueller-Hinton broth. Different concentrations of EryB were tested on planktonic cells (0.01 mM; 0.05 mM; 0.1 mM). The samples were irradiated with a green laser ($\lambda = 532$ nm, 100 mW) for 2 min, 10 min, and with green LED light (2.42 mW) for 30 min, 1 h, 1.5 h, 2h, 2.5 h. The results were assessed by calculating the colony-forming units (CFU/mL). Then, experiments were conducted using a nanocomposite containing the photoactive molecule EryB.

EryB at a concentration of 0.05 mM showed the highest inhibitory effect on the growth of both planktonic and biofilm cells, reducing their survival by 10,000-fold, using both green Led light (1.5 h) and green laser (10 min) compared to control samples representing the growth of bacteria without EryB. The inhibitory effect of EryB without irradiation was also observed, but the growth of both planktonic and biofilm cells was inhibited 100-fold compared to the control samples without EryB. The hybrid film with EryB achieved an approximately 10,000- and 1,000-fold reduction in biofilm growth after irradiation with green LED light (1.5 h) or green laser (10 min), respectively.

In summary, the presented nanocomposite represents a promising approach for further studies considering the potential of modified polymers for various applications, especially in healthcare, requiring specific surface properties.

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LIGHT-ACTIVATED NANOCOMPOSITE ERADICATES MIXED *CANDIDA ALBICANS*–*STAPHYLOCOCCUS AUREUS* BIOFILM

H. Bujdáková^{1*}, J. Czucz Varga¹, J. Bujdák^{2,3}

¹ Department of Microbiology and Virology, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15, Bratislava, Slovakia

² Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15, Bratislava, Slovakia

³ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dubravská cesta 9, 845 36, Bratislava, Slovakia

* helena.bujdakova@uniba.sk

KEYWORDS: Film | Mixed Biofilm | Nanocomposite | Microorganisms

Candida albicans and *Staphylococcus aureus* can cause severe life-threatening infections. The increasing prevalence of antimicrobial resistance underlines the need for alternative therapeutic approaches. Photodynamic inactivation (PDI) has emerged as a promising method for eradication of microbial biofilms. The presented work evaluated the antimicrobial activity of a polyurethane (PU) modified with thin film based on clay mineral saponite modified with inorganic surfactant and with immobilized photoactive dye phloxine B (PhB). Results showed a significant reduction in the survival of both representatives in biofilm after PDI. Scanning electron microscopy confirmed not only killing effect of nanocomposite after PDI, but reduction in the yeast-to hyphae transformation was observed as well. Furthermore, the expression of the *ALS3* and *HWP1* genes in *C. albicans* biofilms was evaluated after PDI. It was proven that after PDI, only the *HWP1* gene was upregulated. Expression of the *ALS3* gene was downregulated or expression was not significantly changed compared to the control sample that was represented by PU alone.

In conclusion, PDI when incorporated into a PU-organoclay nanocomposite demonstrated excellent anti-biofilm activity against dual-species biofilms of *C. albicans* and *S. aureus*. These findings highlight the potential of PDI as an effective alternative strategy for managing resistant biofilms.

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LABORATORY TECHNOLOGICAL RESEARCH OF DOLOMITE FROM SLOVAK DEPOSITS

Z. Danková^{1*}, A. Bekényiová¹, Z. Kollová¹, E. Fedorová¹, P. Bačo¹, J. Briančin²

¹ State Geological Institute of Dionýz Štúr, Regional centre Košice, Jesenského 8, 040 01, Košice, Slovak Republic

² Institute of Geotechnics, Slovak Academy of Sciences, Watsonova 45, 040 01, Košice, Slovak Republic

* zuzana.dankova@geology.sk

KEYWORDS: Dolomite | Annealing | Magnesium metal

At present, China is the largest producer and exporter of magnesium in the world, accounting for more than 85 % of the world's magnesium outputs [1, 2].

In order to ensure within the EU, preferably, self-sufficiency, a stable supply of the essential mineral raw materials required for industry led to the establishment of the European Raw Materials Alliance (ERMA). One of the key objectives is access to sustainable raw materials, as well as support for exploration and mining of raw materials within the EU. The magnesium metal has a special status between 26 elements and minerals defined as “critical raw materials for the EU” and has been included in the list of critical minerals for European Union countries since 2011 [3].

Magnesium is produced by two principal processes: electrolysis of molten magnesium chloride and thermal reduction of magnesia (Pidgeon method) [4].

The most suitable raw material for the MgO production for method of silicothermic reduction is dolomite or magnesite [5]. For technological research, samples from different Slovak deposits (Sedlice, Trebejov, Kraľovany and Stráňavy) were chosen. The samples were annealed at selected temperatures and characterized by thermogravimetry differential thermal analysis (TG/DTA). The results pointed at the different hydration activity of studied samples, which may correspond with their different reduction activity/active sites in their structure to increase the reduction of magnesium.

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LABORATORY TECHNOLOGICAL RESEARCH OF QUARTZITE SAMPLES FROM THE LOCALITY KRNČA

E. Fedorová^{1*}, Z. Danková¹, A. Bekényiová¹, Z. Kollová¹, P. Bačo¹, J. Briančin²

¹ State Geological Institute of Dionýz Štúr, Regional centre Košice, Jesenského 8, 040 01, Košice, Slovak Republic

² Institute of Geotechnics, Slovak Academy of Sciences, Watsonova 45, 040 01, Košice, Slovak Republic

* erika.fedorova@geology.sk

KEYWORDS: Quartz | Technological process | XRD analyse

In Slovakia, the quartz raw materials are relatively well known, being applicable as starting materials for a wide range of practical uses. From the viewpoint of the quartz raw materials use for the production of high-purity SiO₂ raw material, in the conditions of the Slovak part of the Western Carpathians, the deposits of vein quartz in the Gemeric unit are of high perspectives [1].

The preparation of high SiO₂ quartz products using different treatment methods, processes, or their combinations from vein quartz, quartzite, and wind-blown quartz sands was verified. It was found that after grain size treatments, electromagnetic separation, acid leaching (in HCl or HF) and calcination (at 1000 °C), product purities of up to 99.98% SiO₂ (without loss by annealing) were achieved [1].

The metallurgical importance of Si is in the production of some special alloys. The best known is ferrosilicon (an alloy of silicon with iron), which is characterized by high hardness and chemical resistance. Silicon metal is a component of aluminum alloys and is used in the chemical industry to make silicones. It is also popular in the electronics industry and the solar energy sector (solar panels, silicon chips, semiconductors). It improves the properties of aluminium such as strength, hardness or fluidity. The addition of silicon metal makes aluminium alloys strong and lightweight. Silicon metals are also useful in the automotive industry as a replacement for heavier parts made from cast iron. Alloy wheels and engine blocks are vehicle parts that are very often produced as aluminium castings with the addition of silicon. Silicon metal is a key raw material for many industries. Without silicon, we would not be able to use computers, solar panels and many building products [2].

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THE CRITICAL AND STRATEGIC RAW MATERIALS OF THE EU AND THEIR POTENTIAL IN SLOVAKIA

Z. Kollová^{1*}, P. Bačo¹, Z. Danková¹, Z. Németh¹

¹ State Geological Institute of Dionýz Štúr, Regional centre Košice, Jesenského 8, 040 01, Košice, Slovak Republic

* zuzana.kollova@geology.sk

KEYWORDS: Critical and strategic raw materials | Potential in Slovakia

The situation regarding the availability of raw materials led to the development of the Regulation (EU) 2024/1252 of the European Parliament and of the Council establishing a framework for ensuring a secure and sustainable supply of critical raw materials [1]. The new regulation sets out a series of comprehensive measures to ensure the European Union's access to secure, diversified, affordable and sustainable supplies of critical raw materials. This is essential for Europe's competitiveness, including in green and digital industries, as well as defence and aerospace, according to a European Commission report. The EU should have the capacity to extract 10%, process 40% and recycle 25% of its annual consumption of strategic raw materials within the EU by 2030, according to the agreed benchmarks.

Slovakia is currently completing National Exploration Programme based on knowledge of the metallogenetic development of the territory, focusing on potentially significant sources of selected CRM. Information on the availability of the CRM, which are essential for industrial production in the Slovak Republic, but also in the EU countries in general, has recently been processed in several geological synthesis works [2 - 4].

The number of CRMs is constantly increasing, which means that their provision for the needs of the EU economy remains essential. An assessment of the potential of the Slovak Republic from the perspective of CRMs for the EU [5] pointed out the possibilities of using domestic raw materials.

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PREPARATION AND CHARACTERIZATION OF TRIMETHYL CHITOSAN - SMECTITE NANOCOMPOSITES

V. Kureková^{1*}, D. Kováčik², K. Bilská³, H. Bujdáková³, F. Gread⁴, M. Osacký⁴, M. Pribus¹

¹ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

² Department of Experimental Physics, Faculty of Mathematics, Physics and Informatics, Comenius University, Mlynská dolina F1, 842 48, Bratislava, Slovakia

³ Department of Microbiology and Virology, Faculty of Natural Sciences, Comenius University, Ilkovičova 6, 842 15, Bratislava, Slovakia

⁴ Department of Mineralogy, Petrology and Economic Geology, Faculty of Natural Sciences, Comenius University, Ilkovičova 6, 842 15, Bratislava, Slovakia

* valeria.kurekova@savba.sk

KEYWORDS: N,N,N-trimethyl chitosan | Layer charge | Layer-by-layer method | FTIR spectroscopy

N,N,N-trimethyl chitosan (TMCH) is an antibacterial, biocompatible, biodegradable and highly bioadhesive polymer in comparison to chitosan (CH). TMCH and/or CH, along with two smectites with different cation exchange capacity (CEC), were used for the preparation of hybrid systems using the layer-by-layer (LBL) method. The objective of this work was to study the influence of the smectite layer charge on the resulting properties of hybrid systems. For the preparation of hybrid films, Sumecton SA (S; CEC = 0.72 mmol/g) and montmorillonite Lutilla from a new Slovak deposit (Lu; CEC = 1.14 mmol/g) smectites were used. The polypropylene glass (PP), used as a substrate for LBL films, was activated by DCSBD plasma for 20 s in ambient air and then put into TMCH or CH solution. After the activation, the PP was immersed in stock solutions of S or Lu, followed by immersion in TMCH or CH solution. This constituted the first layer of the LBL film. Films were prepared by alternating layers of cationic CH and TMCH molecules with negatively charged S and Lu until a total of 40 layers of the LBL film was reached. Infrared spectra were measured by the ATR method after the deposition of each layer. The most significant changes were observed in the 950 – 1100 cm⁻¹ region. These changes were attributed to Si-O stretching vibrations of smectites and C-O stretching vibrations of CH and/or TMCH. The intensity of the bands increased linearly up to 25 layers, after which the growth stopped. For this reason, the PP glass with 20 layers was reactivated by DCSBD plasma. After this step, the layers increased linearly up to the applied 40 layers. As the number of layers increased, the following trend was observed in the intensity of the band region: TMCH-S < CH-S < TMCH-Lu < CH-Lu. To increase the quantity of TMCH in LBL samples, 1 wt. % of CH₃COOH was also used for film preparation. This modification helped to increase the amount of TMCH; the band intensities were approximately the same as those of the CH samples. From these results, the influence of the layer charge on the sample properties is obvious; films prepared with Lu (higher CEC) contained higher amounts of components compared to S. The antibacterial activity of the prepared samples was also tested. The most pronounced bacterial inhibition was observed for the TMCH-Lu sample and confirmed the substantial influence of layer charge and type of polymer on the resulting properties of the materials.

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IR SPECTROSCOPIC CHARACTERIZATION OF NATURAL AND ORGANO-MODIFIED MONTMORILLONITE FROM THE SLOVAK BENTONITE DEPOSIT LUTILA

J. Madejová^{1*}, P. Boháč¹, L. Jankovič¹, V. Kureková¹, M. Osacký², P. Uhlík²

¹ Department of Hydrosilicates, Institute of Inorganic Chemistry Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

² Department of Mineralogy, Petrology and Economic Geology, Faculty of Natural Sciences, Comenius University, Ilkovičova 6, 842 15, Bratislava, Slovakia

* jana.madejova@savba.sk

KEYWORDS: Bentonite | Organic cations | IR spectroscopy

Bentonite is unique raw industrial material due to broad range of its possible industrial and environmental applications. With annual production ~300 kt of bentonite, Slovakia belongs to the top 10 world's countries in bentonite. One of the relatively newly-opened bentonite deposit in Slovakia is Lutilla I, located in the south-western part of the Kremnické vrchy Mts. The fine fraction of bentonite from deposit Lutilla (Na-Mnt) and its organo-modified forms (O-Mnts) were thoroughly studied by different experimental techniques including IR spectroscopy.

The IR spectrum of Na-Mnt revealed the characteristic absorption bands of a montmorillonite; the OH stretching band near 3630 cm⁻¹, the OH bending bands in the 920-840 cm⁻¹ region and the Si-O-Al and Si-O-Si near 524 and 468 cm⁻¹. The IR spectra of O-Mnts, prepared by intercalation of dioctylammonium (2C8) and hexadecylammonium (1C16) cations, showed the absorption bands related to the stretching (3000-2800 cm⁻¹) and deformation (1500-1400 cm⁻¹) vibrations of the CH₃ and CH₂ groups as well as stretching (3300-3200 cm⁻¹) and deformation (1550-1400 cm⁻¹) vibrations of the NH₂ and NH groups. With increasing amount of the organic cations, the intensity of the C-H and N-H bands increased. The position of the CH₂ stretching band was used for determining the arrangement of organic cations occurring in the interlayers of Mnt. The band was gradually shifted from a position characteristic for prevailing disordered *gauche* conformers (2931 cm⁻¹ for 2C8 and 2925 cm⁻¹ for 1C16) to lower wavenumbers (2927 cm⁻¹ for 2C8 and 2918 cm⁻¹ for 1C16) indicating an increasing number of ordered all-*trans* conformers.

Detailed characterization of prepared materials is an essential step to change the current traditional processing technology of Lutilla I bentonite into new, innovative and value-added applications.

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CHARACTERIZATION OF ALBERTA OIL SANDS MATURE FINE TAILINGS

M. Osacký^{1*}, Y. Bai¹, H. Pálková², P. Uhlík¹

¹ Department of Mineralogy, Petrology and Economic Geology, Faculty of Natural Sciences, Comenius University, Ilkovičova 6, 842 15, Bratislava, Slovakia

² Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

*osacky@fns.uniba.sk

KEYWORDS: Oil sands | Tailings | Bitumen extraction

The Alberta oil sands deposit represents the fourth largest reserve of oil on the planet. Commercial separation of bitumen from the oil sands is achieved by hot water based extraction (WBE). One of the most significant shortcomings of WBE is production of large volumes of waste, known as tailings, which consist of sand, silt, clays, unrecovered bitumen and water. Tailings from the extraction process are deposited in tailings ponds where coarse sands settle quickly to the bottom whereas smaller particles (mostly clays and clay minerals) remain suspended in water for long periods, forming fluid fine tailings. After a few years of settling, stable and viscous gel-like suspension called mature fine tailings (MFT) is formed. The consolidation rate of MFT is extremely slow and without intervention it may take decades to centuries. However, eventually all tailings must be reclaimed and integrated into mine closure landforms in a timely manner to meet regulatory requirements. Currently, the dewatering and consolidation of oil sands tailings is likely the most challenging problem faced by the oil industry. Despite great efforts of industry and academia, the commercial technology for fast, efficient and economic dewatering and consolidation of oil sands tailings has not yet been developed. Although it is generally believed that clay minerals and/or residual bitumen may be largely responsible for slow dewatering and low consolidation rates of oil sands tailings their particular role on the dewatering and consolidation of tailings is still poorly understood.

In order to better understand the role of clay minerals and residual organics on settling behavior of MFT, set of settling experiments was performed in the present study. Contrary to the previous works where various MFT size fractions were typically characterized upon their isolation from the bulk sample, in the present study, distinct settling layers, naturally occurring during settling of bulk MFT under laboratory conditions, were collected and analyzed. To evaluate the impact of residual organics on settling behavior of oil sands tailings, settling of untreated MFT was compared with the settling of MFT samples after applying two different procedures to extract the residual bitumen (solvent-based and bleach-based extraction). The ability to adsorb and release water for distinct settling layers was also investigated.

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SILICA NETWORK DEVELOPMENT VIA SILANE HYDROLYSIS IN COMPOSITE BASED ON ORGANOMODIFIED HECTORITE

H. Pálková^{1*}, J. Madejová¹, M. Zimowska²

¹ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36 Bratislava, Slovakia

² Jerzy Haber Institute of Catalysis and Surface Chemistry, PAS, Niezapominajek 8, 30-239 Krakow, Poland

* helena.palkova@savba.sk

KEYWORDS: Hectorite | Organic modification | Silane | Infrared spectroscopy

Study presents a comprehensive investigation of Laponite-derived porous clay heterostructures (PCHs), emphasizing the role of tetraethylorthosilicate (TEOS) in the formation of mesoporous silica frameworks and the application of FTIR spectroscopy for structural analysis. The synthesis strategy involved intercalation of hexadecyltrimethylammonium (HDTMA⁺) surfactants and neutral dodecylamine (DDA) into synthetic hectorite, followed by TEOS hydrolysis to create a silica network between the exfoliated clay layers. The materials were characterized through a combination of solid-state ²⁹Si MAS NMR and FTIR spectroscopy in both middle and near-infrared regions (MIR and NIR). ²⁹Si MAS NMR confirmed formation of the silica network developed upon hydrolysis and Q⁴ centres and surface Q³ Si sites were detected in the spectra.

FTIR spectroscopy proved crucial for tracking structural transformations throughout the synthesis. Upon addition of co-surfactant DDA and Si-source (TEOS) to HDTMA-Laponite a broad complex Si–O band at 1070 cm⁻¹ appears, evidencing the hydrolysis of TEOS and development of silica network in the PCH-precursor. The NIR spectrum shows characteristic O–H and C–H bands of HDTMA-Laponite and the N–H overtones (6523 and 6478 cm⁻¹) and combination (4935 cm⁻¹) band of dodecylamine. Only this region permits identification of NH₂ groups because the N–H bands in the MIR region are overlapped with absorption bands of water molecules. No C–H or N–H vibrations relating to organic template could be recognized in the NIR spectrum after PCH-precursor calcination. Laponite component in the calcined PCH-precursor, as final step of synthesis retains its layered structure, as evidenced by the presence of Mg₃OH and Si–O bands in the spectra. In addition, PCH material contained SiOH groups of different local environment, the feature that can be very useful in adsorption processes.

Both complementary methods provided a consistent picture of the mechanism by which silane-derived silica networks assemble within Laponite hosts and confirmed their effectivity in monitoring of structural evolution during composite material syntheses.

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IMMOBILIZATION OF 1,10-PHENANTHROLINE BY MONTMORILLONITE – DFT STUDY

E. Scholtzová^{1*}, E. Mičejová²

¹ Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

² Department of Inorganic Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15, Bratislava, Slovakia

* eva.scholtzova@savba.sk

KEYWORDS: 1,10-Phenanthroline | Montmorillonite | Smectite clay | DFT

1,10-Phenanthroline (phen), a classic chelating bidentate ligand for transition metal ions, is essential in developing coordination chemistry [1] and as a rigid, planar, hydrophobic heteroaromatic ligand containing nitrogen atoms cooperating in cation coordination forms stable coordination complexes. Metal–phen complexes often exhibit unique properties such as strong luminescence, for example. Due to its widespread use as a chelating agent, phenanthroline and its derivatives are repeatedly detected as trace contaminants in wastewater. Clay minerals are abundant, naturally occurring, and cost-effective materials widely used in remediation technologies. Their valuable properties, such as high specific surface area, significant porosity, intrinsic surface charge, and diverse surface functional groups, contribute to their effectiveness as adsorbents, filtration media, flocculants, and carbon stabilizers. Moreover, the surface properties of clay minerals can be modified from hydrophilic to hydrophobic, enhancing their capacity to adsorb and transport non-ionic organic compounds in aqueous systems. [2].

This study used montmorillonite clay as a model structure to evaluate the stability of phenanthroline–smectite hybrid material as a prospective material for phen immobilization. The potential of these materials for further technological applications, such as in environmental sensing, pollutant removal, and adsorption processes, is very promising. The density functional theory (DFT) method with the D3 scheme [3] for dispersion corrections implemented in the VASP program was used for structure examination. The findings highlight the stability of the studied phen–montmorillonite hybrid structure.

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PHYSICO-CHEMICAL CHARACTERIZATION OF A THIOL-FUNCTIONALIZED MONTMORILLONITE/BIOCHAR COMPOSITE

M. Slaný^{1,2*}

¹ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

² Department of Materials Engineering and Physics, Faculty of Civil Engineering, Slovak University of Technology, Radlinského 11, 810 05, Bratislava, Slovakia

* michal.slany@savba.sk

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In this study, a thiol-functionalized montmorillonite/biochar composite was synthesized using a hydrothermal process. The composite was prepared by incorporating thiol groups (3-Mercaptopropyl)trimethoxysilane (MPTMS) into the montmorillonite in the presence of biochar, under controlled hydrothermal conditions.

Structural analysis was conducted using XRD and FTIR to determine crystallinity and functional groups in the composite. SEM provided insights into the morphology, while TGA/DSC assessed the composite's thermal stability.

The XRD analysis revealed the amorphous nature of biochar, as evidenced by a broad diffraction peak around 2θ values of $20\text{--}30^\circ$, indicative of its lack of long-range order. In contrast, the montmorillonite component showed distinct crystalline peaks, confirming its structural integrity. FTIR spectroscopy confirmed the successful functionalization of the montmorillonite/biochar composite with MPTMS. The thiol group ($-\text{SH}$) showed absorption band at 2550 cm^{-1} , and the alkyl chains ($-\text{CH}_2-$) exhibited stretching vibrations around 2850 cm^{-1} and 2920 cm^{-1} , confirming the presence of MPTMS in the composite [1]. TGA/DSC analysis revealed the thermal stability and decomposition behavior of the thiol-functionalized montmorillonite/biochar composite. Weight loss around $100\text{--}150\text{ }^\circ\text{C}$ indicated water removal, while a further loss between $300\text{--}500\text{ }^\circ\text{C}$ was due to the decomposition of organic components, including alkyl and thiol groups from MPTMS. A distinct weight loss around $600\text{--}800\text{ }^\circ\text{C}$ corresponded to the dehydroxylation of montmorillonite. The SEM analysis revealed uniform dispersion of biochar particles within the montmorillonite matrix, with slight aggregation due to interactions between biochar and silane groups. Functionalization with (3-MPTMS) resulted in more compact surface structures, indicating successful thiol group incorporation.

The thiol-functionalized montmorillonite/biochar composite exhibits successful structural and chemical modifications, enhancing its potential for adsorptive applications. The functionalization with thiol groups suggests it may be effective in removing specific pollutants.

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HYBRID SYSTEMS BASED ON LAYERED SILICATE NANOPARTICLES AND LUMINESCENT IRIDIUM(III) COMPLEXES

T. Šimonová^{1*}, J. Bujdák^{1,2}, P. Hrobárik³

¹ Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

² Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15, Bratislava, Slovakia

³ Department of Inorganic Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15, Bratislava, Slovakia

* timea.simonova@savba.sk

KEYWORDS: Adsorption-induced emission | Cyclometalated Ir(III) complexes | Smectites | Phosphorescence

Phosphorescent Ir(III) complexes are widely studied for their electrochemical and photophysical properties, enabling uses in optoelectronics, photocatalysis, and photodynamic therapy. Our research focuses on $[\text{Ir}(\text{2-phenylpyridine})_2(\text{2,2'-dibenzothiazole})][\text{PF}_6]$ (IrC), a red-light-emitting cationic luminophore from the $[\text{Ir}(\text{C}^{\wedge}\text{N})_2(\text{N}^{\wedge}\text{N})]^+$ group [1].

Hybrid systems of IrC with layered silicate nanoparticles were prepared to study how adsorption influences the photoactivity of the complex cations. We investigated the effect of surface concentration of adsorbed IrC molecules (a_{IrC}) on photophysical properties across various smectite dispersions, varying structure, particle size, and surface charge. The IrC concentration was constant in each dispersion, while different a_{IrC} values were achieved by varying the ratio of the amount of IrC molecules to the mass of smectite. Absorption and luminescence properties were investigated using UV-Vis absorption and fluorescence spectroscopy and time-resolved luminescence measurements. IrC showed a large Stokes shift and emitted in the red to near-infrared region. Interaction with silicate particles increased both luminescence intensity and excited-state lifetime of the IrC cation in the dispersions of all selected smectites. The most significant enhancement, a 24.7-fold increase in IrC emission intensity compared to its solution, occurred in saponite Sumecton dispersions at the lowest a_{IrC} (0.48% of cation exchange capacity (CEC)). This suggests that the adsorption of IrC molecules onto silicate surfaces suppresses non-radiative relaxation, indicating adsorption-induced emission phenomenon. While the emission intensity increase slightly decreased with higher a_{IrC} , the effect of surface concentration was generally minor; significant luminescence enhancement was still observed even at high surface concentrations (89.7% of CEC), where the presence of photophysical interactions between adsorbed molecules can be assumed.

In summary, the preparation of hybrid dispersions of smectite nanoparticles with cationic Ir(III) complexes is a promising strategy to enhance the phosphorescence quantum yield of these luminophores.

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A HYDRATION, DEHYDRATION AND DEHYDROXYLATION OF BENTONITE FROM LUTILA I DEPOSIT

P. Uhlík^{1*}, F.A. Gread¹, B. Guspan¹, H. Pálková², J. Brčeková¹, M. Osacký¹

¹ Department of Mineralogy, Petrology and Economic Geology, Faculty of Natural Sciences, Comenius University, Ilkovičova 6, 842 15, Bratislava, Slovakia

² Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

* peter.uhlik@uniba.sk

KEYWORDS: Montmorillonite | Molecular and hydroxyl water | Swelling | Thermal analysis

The main subjects of the research were two commercial bentonite samples from the Lutilla I deposit, Kremnické vrchy. The RLU sample was Na-activated bentonite from Romin Slovakia, spol. s r. o. and the ELU sample was natural Ca-Mg-bentonite, (Envigeo, a.s.). Both samples were ground and dried with a particle size of <63 µm. A swelling test was performed on these samples and after heating, 105 °C, 200 °C, 400 °C and 800 °C - the swelling index of bentonite was determined according to the ASTM-DM890 standard.

The swelling factor at room temperature of 25°C was 2.5 for the ELU sample and up to 12.2 for the RLU sample. The increase in swelling indicated an improvement in the properties of bentonite that had undergone drying at 105°C and 200°C. The calcination process led to partial dehydroxylation at 400°C, which was indicated by an increased weight change, shrinkage, and reduced swelling ability. The ELU sample did not swell at all. The higher thermal stability for RLU at 400°C was also confirmed by XRD. Complete dehydroxylation most likely occurred at 800°C, which was reflected by greater water release, inability to swell and complete disappearance of montmorillonite peaks in XRD patterns. Based on the weight change, it was observed that a significant dehydroxylation step occurred at a temperature lower than 800°C, since there was only a small difference in weight change between 600°C and 800°C.

The amount of moisture lost (molecular water) from the RLU sample was approximately 6.8% of the original weight after drying at 105 °C, while the ELU showed more than twice the moisture loss, meaning that the moisture was about 12% of the weight before analysis. Almost twice the amount of water content was removed during the drying process for the ELU bentonite sample containing hydrated divalent calcium and magnesium cations with two layers of water compared to the RLU bentonite sample with hydrated monovalent sodium cations, which contained only one layer of water molecules.

Thermal analysis was also applied to a set of bentonite samples from the Bartošova Lehôtka II and Lastovce deposits. The samples from Bartošova Lehôtka II showed dehydroxylation maxima around 700 °C, indicating a predominance of the cis-vacant variant of octahedral sites. In contrast, most of the samples from Lastovce showed bimodal dehydroxylation curves, indicating the presence of both cis and trans-vacant variants of dioctahedral smectite.

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LIST OF PARTICIPANTS

1.	ASBAT AYESHA	Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
2.	BASHIR SANAM	Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
3.	BERSHADSKYI ANTON	Department of Materials Engineering and Physics, Faculty of Civil Engineering, Slovak University of Technology, Bratislava, Slovakia
4.	BEKÉNYIOVÁ ALEXANDRA	Department of Applied Technology of Raw Minerals, State Geological Institute of Dionýz Štúr, Košice, Slovakia
5..	BILSKÁ KATARÍNA	Department of Microbiology and Virology, Faculty of Natural Sciences, Comenius University in Bratislava, Bratislava, Slovakia
6.	BOHÁČ PETER	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
7.	BÖSERLE HUDCOVÁ BARBORA	Department of Environmental Geosciences, Faculty of Environmental Sciences, Czech University of Life Sciences, Prague, Czech Republic
8.	BUDZÁK ŠIMON	Department of Chemistry, Faculty of Natural Sciences, Matej Bel University, Banská Bystrica, Slovakia
9.	BUGYNA LARYSA	Department of Microbiology and Virology, Faculty of Natural Sciences, Comenius University in Bratislava, Bratislava, Slovakia
10.	BUJDÁK JURAJ	Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Bratislava, Slovakia
11.	BUJDÁKOVÁ HELENA	Department of Microbiology and Virology, Faculty of Natural Sciences, Comenius University in Bratislava, Bratislava, Slovakia
12.	DANKOVÁ ZUZANA	Department of Applied Technology of Raw Minerals, State Geological Institute of Dionýz Štúr, Košice, Slovakia
13.	FEDOROVÁ ERIKA	Department of Applied Technology of Raw Minerals, State Geological Institute of Dionýz Štúr, Košice, Slovakia
14.	GEORGE VINNY	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
15.	CHYSTIAKOV ARTEM	Department of Materials Engineering and Physics, Faculty of Civil Engineering, Slovak University of Technology, Bratislava, Slovakia
16.	KLEMAN SANTOS LEONARDO FILIPE	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
17.	KOLLOVÁ ZUZANA	Department of Raw Minerals and Geophysics, State Geological Institute of Dionýz Štúr, Košice, Slovakia
18.	KUREKOVÁ VALÉRIA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
19.	LABIB SHOTORBAN PARISA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
20.	LABUTA JÁN	Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, Czech Republic
21.	MADEJOVÁ JANA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
22.	OSACKÝ MAREK	Department of Mineralogy, Petrology and Economic Geology, Faculty of Natural Sciences, Comenius University, Bratislava
23.	PÁLKOVÁ HELENA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava
24.	PINZÓN DANIEL	Department of Mineralogy, Petrology and Economic Geology, Faculty of Natural Sciences, Comenius University, Bratislava
25.	PLANETOVÁ VIKTÓRIA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava
26.	SCHOLTZOVÁ EVA	Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava
27.	SLANÝ MICHAL	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak

	Academy of Sciences, Bratislava
28. ŠIMONOVÁ TÍMEA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava
29. ŠKORŇA PETER	Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava
30. UHLÍK PETER	Department of Mineralogy, Petrology and Economic Geology, Faculty of Natural Sciences, Comenius University, Bratislava

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