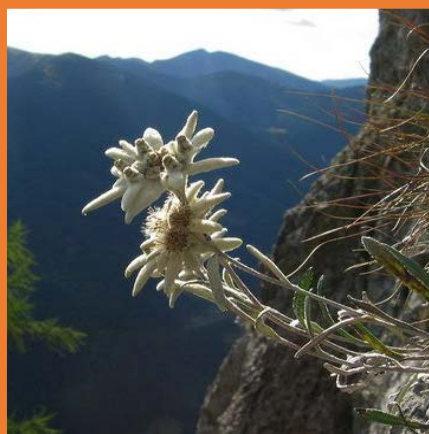


# 10<sup>th</sup> WORKSHOP OF SLOVAK CLAY GROUP



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

BOOK OF ABSTRACTS



JUNE 24 – 26, 2024, TATRANSKÁ LOMNICA, SLOVAKIA



10<sup>th</sup> Workshop of Slovak Clay Group

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MATERIAL SCIENCE, APPLICATIONS, AND  
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# ORAL PRESENTATIONS





# MECHANICAL PROPERTIES OF SMECTITE CLAYS AND CLAY-POLYMER HYBRIDS BY DFT-D3 METHOD

S. Bashir<sup>1\*</sup>, E. Scholtzová<sup>1</sup>, D. Tunega<sup>2</sup>

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

<sup>2</sup> Institute of Soil Research, Department of Forest- and Soil Sciences, University of Natural Resources and Life Sciences, Peter-Jordan-Strasse 82b, A-1190, Wien, Austria

\* [sanam.bashir@savba.sk](mailto:sanam.bashir@savba.sk)

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**KEYWORDS:** Smectites | Clay-polymer hybrids | Elastic constants | DFT-D3 method

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In the past two decades, hybrid materials have gained popularity due to their enhanced mechanical properties. Polymers, known for their low mechanical strength, can significantly benefit from the incorporation of small amounts of clay minerals [1]. However, due to the small size of clay minerals and the complexity of their interfacial interactions with polymers, experimental methods alone may not accurately determine specific mechanical properties [2].

This study employed a theoretical computational approach to analyze the mechanical properties of studied smectite clay minerals and their hybrids with poly(2-methyl-2-oxazoline) (PMeOx) polymer. The structural stability and mechanical properties of four smectite clay minerals—montmorillonite, beidellite, saponite, and hectorite were analyzed individually. Subsequently, PMeOx pentamer were intercalated into the interlayer space of the studied smectites to form clay-polymer hybrids, which were then analyzed for their structural stability and mechanical properties. Elastic constants were determined using the stress-strain approach *via* DFT-D3 methods. From these constants, elastic moduli, including bulk modulus ( $K_{VRH}$ ), shear modulus ( $G_{VRH}$ ), Young's modulus ( $E_{VRH}$ ), and Poisson's ratio ( $\nu$ ), were calculated using the Voigt-Reuss-Hill approximation [3]. The findings confirmed the stability of PMeOx with all studied smectite clays and highlighted differences in structural stability and mechanical properties between dioctahedral (montmorillonite and beidellite) and trioctahedral (saponite and hectorite) smectites, with the trioctahedral smectites and their hybrids showing superior properties.

Trioctahedral smectites and their hybrids exhibited higher structural stability and better mechanical properties due to their rigid and compact structures. Among these, hectorite displayed the highest structural stability and mechanical properties when combined with PMeOx. This study provides valuable insights into the interactions and stability of the clay-polymer hybrid materials.

## Acknowledgment:

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# PHOTOACTIVE NANOCOMPOSITE SYSTEM BASED ON CLAY MINERAL SAPONITE EFFECTIVELY ERADICATES STAPHYLOCOCCAL BIOFILMS

**K. Bilská<sup>1\*</sup>, L. Bugyna<sup>1</sup>, M. Pribus<sup>2</sup>, J. Bujdák<sup>2,3</sup>, H. Bujdáková<sup>1</sup>**

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

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

<sup>3</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

\* bilska6@uniba.sk

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**KEYWORDS:** Nanocomposite | *Staphylococcus* | Antibiofilm | Photoactive

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*Staphylococcus aureus* is a bacterium that has been found for several years on WHO (World Health Organization) bacterial priority pathogens list as high-priority pathogen, due to global threat, persistence prevalence, biofilm formation, and multi-drug resistance, especially methicillin-resistant *S. aureus* (MRSA) strains. The formation of staphylococcal biofilms on medical devices are connected to problematic treatment of infections.

In this study, polyurethane (PU) material modified with a nanocomposite based on the clay mineral saponite (Sap) and poly(diallyldimethylammonium) (PDDA) (1.5 mmol/g) functionalized with photoactive compounds phloxine B (PhB) and erythrosin B (EryB) were used (1.5 mmol/g). During experimental work, standard strain *Staphylococcus aureus* CCM3953 and clinical isolates *S. aureus* S61 and L12 were used. The effectiveness of the material was tested on 24-h biofilms before and after irradiation with a green laser (IR;  $\lambda = 532$  nm, 100 mW, duration of irradiation for 120 s). The biocompatibility of individual components of the nanocomposite (Sap 0.1 g/L; PDDAC 0.05 wt. %; PhB and EryB 0.5 mM) was tested *in vivo* on *Galleria mellonella* model for 10 days. The effectiveness of photoactive PhB (0.05 mM) was tested on *ex vivo* model of mice tongues growth with 72-h *S. aureus* biofilms and evaluated by light and fluorescence microscopy.

The PU material with PhB showed higher effectiveness against staphylococcal biofilms compared to PU with EryB. The PU with PhB achieved on a log scale 2.82 inhibition after 2 min of IR, while PU with EryB demonstrated on a log scale 0.86 inhibition after 2 min of IR. Nanocomposite with EryB achieved the same effect as PhB material after 10 min of IR with green laser (on a log scale 2.77 inhibition). Nanocomposite system with PhB confirmed the effectiveness against MRSA L12 and S61 strains too. Experiments on *G. mellonella* model did not showed toxicity of individual components of material for 10 days. Microscopy of mice tongues showed strong decrease of 72-h biofilms on the surface of tissue after usage of PhB and IR with green laser.

The results of the study showed photoactive nanocomposite nanomaterials as effective system for eradication of staphylococcal biofilms and confirmed their potential for other research and development of more advanced material for medical field.

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# ADSORPTION INDUCED LUMINESCENCE: INSIGHTS FROM THEORY

Š. Budzák<sup>1\*</sup>, P. Boháč<sup>2</sup>, M. Pribus<sup>2</sup>, V. Planetová<sup>2</sup>, J. Bujdák<sup>2,3</sup>

<sup>1</sup> Department of Chemistry, Faculty of Natural Sciences, Matej Bel University, Tajovského 40, 97401, Banská Bystrica, Slovakia

<sup>2</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 84536, Bratislava, Slovakia

<sup>3</sup> Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 84215, Bratislava, Slovakia

\* [simon.budzak@umb.sk](mailto:simon.budzak@umb.sk)

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**KEYWORDS:** Fluorescence | Adsorption | Density Functional Theory | Conical Intersection

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Compared to ground-state reactions and phenomena, excited-state chemistry is more challenging to study with standard experimental tools. There are no X-ray or NMR methods to characterize the structure of larger organic molecules in the short timeframes following electron excitation. However, fluorescence and its changes, singlet oxygen generation, excited-state proton transfer, and other photochemical changes are intensively studied since light is a high-energy source capable of very specific actions [1].

In our contribution, we show how theoretical chemistry can complement experimental findings. Using three different case studies [2-4], we will demonstrate the strengths of excited-state calculations, but we will also highlight the limitations and properties that remain difficult to calculate. In the context of clay research, we will demonstrate how different surfaces can support fluorescence turn-on by hindering non-radiative pathways.

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# ANTIMICROBIAL SURFACES OF POLYMERS IN THE FORM OF THIN COMPOSITE ACTIVE LAYERS

J. Bujdák<sup>1,2\*</sup>, E. Skoura<sup>2</sup>, N.C.T. Dadi<sup>3</sup>, H. Bujdáková<sup>3</sup>

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

<sup>2</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

<sup>3</sup> Department of Microbiology and Virology, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15 Bratislava, Slovakia

\* juraj.bujdak@uniba.sk

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**KEYWORDS:** Organic dyes | Photo-dissinfection | Photoactivity | Clay/polymer nanocomposites

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Nanocomposites of polymers and clay minerals represent a diverse class of materials used in various applications. Recently, composites with antimicrobial surfaces have attracted considerable interest. Clay mineral particles can effectively serve as carriers for antimicrobial molecules by controlling their gradual release from the polymer matrix or by modifying the surface properties of the polymer composite to achieve the desired effect.

The lecture will start with an overview of the types, preparation strategies and key properties of antimicrobial composites. The second part will focus on specific materials and present the most important results of our ongoing research. A key criterion for the antimicrobial activity of composites is the achievement of a sufficient surface concentration of bioactive molecules. In conventional composites, the effective concentration is often achieved by a high proportion of the functionalized filler, which can impair some of the mechanical properties of the polymer.

The lecture will focus on methods for the synthesis of composites in the form of thin films on the surface of the polymer matrix. This approach offers two main advantages: a high concentration of the active component on the surface and the preservation of the mechanical properties of the polymer matrix. Two systems will be briefly presented, both prepared by combining thin films of organoclay functionalized with the photosensitizer phloxine B and a polymer matrix. In the first system, the composite was formed by reaction with the liquid phase of polyurethane precursors [1]. In the second system, a polycaprolactone melt was used as the liquid phase [2]. In both cases, the liquid phase of the polymer melt or precursor penetrated the organoclay film. This combination resulted in thin composite films several microns thick on the matrix surface without significantly limiting the concentration of the photosensitizer. The presentation will highlight the key properties of these materials, with particular emphasis on their antimicrobial activity.

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# WHAT CAN THE *IN VIVO* MODEL *GALLERIA MELLONELLA* PROVIDE IN THE STUDY OF NANOCOMPOSITES BASED ON CLAY MINERALS AND PHOTOSENSITIZERS?

H. Bujdaková<sup>1\*</sup>, K. Bilská<sup>1</sup>, S. Kendra<sup>1</sup>, L. Bugyna<sup>1</sup>, J. Bujdák<sup>2,3</sup>

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

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

<sup>3</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

\*[helena.bujdakova@uniba.sk](mailto:helena.bujdakova@uniba.sk)

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**KEYWORDS:** *Galleria mellonella* | Nanocomposite | Photodynamic therapy | Organoclay

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Conventional *in vitro* assays fail to mimic true physiological responses of living organisms against nanoparticles or nanocomposites whereas animal *in vivo* models are costly and ethically controversial. Larvae of *Galleria mellonella* are an alternative invertebrate model that provides a platform for testing the biocompatibility of different compounds, the kinetics of survival after an infection followed by subsequent treatment, and for the evaluation of different parameters of host-pathogen interaction. The *G. mellonella* immune response includes cellular and humoral components with structural and functional similarities to the immune effectors found in higher vertebrates, such as humans. However, a limitation is the lack of adaptive immune response. Antimicrobial photodynamic therapy (aPDT) is an alternative approach for combating microbial infections including those associated with biofilm-. The aPDT is effective against Gram-positive and Gram-negative bacteria, viruses, fungi, and parasites. The model *G. mellonella* has been proven to be suitable for the study of aPDT, despite some limitations, for example, the availability of oxygen or the delivery of light into the tissue. The aPDT could be also applicable in the case of testing nanocomposites with photoactive properties. A good example is nanocomposites based on polyurethane modified with organoclay with functionalized phloxine B [1]. All components of the nanocomposite are usually tested alone, but recent testing titanium implants such as K-wire in the *G. mellonella* model showed a direction, how such nanocomposites could be implanted and tested for antimicrobial effect against microbial biofilms [2]. In addition, *G. mellonella* can also provide information about the immune response represented by the production of antimicrobial peptides and also the analysis of hemolymph in the number and representation of hemocytes that varies during the life of the insect and in response to pathogens. Taken together, *G. mellonella* has great potential for different experimental studies focused on microbiological, medical, or pharmaceutical research.

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# HYDROGEL NANOCOMPOSITES WITH ANTIMICROBIAL AND PHOTOACTIVE MOLECULES

V. George<sup>1\*</sup>, P. Boháč<sup>1</sup>, J. Bujdák<sup>1,2</sup>

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

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

\* [vinny.george@savba.sk](mailto:vinny.george@savba.sk)

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**KEYWORDS:** Smectite | Organoclay | Photosensitizer | Hydrogel nanocomposite

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Hybrid materials made of clay minerals and organic dyes have functional advantages and a wide range of possible applications [1]. By incorporating these hybrids into polymers, multifunctional nanocomposites for biomedical applications can be produced [2]. By modifying the surface of a material, the surface properties can be altered without affecting the properties of the polymer bulk, opening up new possibilities for specific applications [3]. In this work, the cationic surfactant hexadecyltrimethylammonium (HDTMA) and the polycation poly(diallyldimethylammonium) PDDA were used to modify synthetic saponite (Sap). The resulting highly hydrophobic organoclay was functionalized with an anionic dye, phloxine B. Thin films were prepared on Teflon membranes using the vacuum filtration method [2]. The objective was to use thin films for the surface modification of hydrogel membranes. The synthesis procedures of different types of hydrogels are about to be tested. The selection of the appropriate polymer would depend on the compatibility with the silicate films to form a nanocomposite layer. One of the tested hydrogels was prepared by radical polymerization of [2-(methacryloyloxy)ethyl]-dimethyl-(3-sulfopropyl)-ammonium hydroxide (sulfobetaine methacrylate ester, SBME), a zwitterionic monomer, using ethylene glycol dimethacrylate (EGDM) as a crosslinking agent. The synthesis of the nanocomposite involves the intercalation of the polymer precursors into the silicate layer, which leads to a modification of the hydrogel with the functionalized organoclay at the interface between the film and the hydrogel. The effects of adsorption time and colloidal stability on the film formation and the properties of the final nanocomposites are analyzed by UV-Vis spectroscopy, fluorescence spectroscopy, and XRD.

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# HALLOYSITE AS SORBENT OF DICLOFENAC FOR PHARMACEUTICAL AND ENVIRONMENTAL USES

**E. Gianni<sup>1,2\*</sup>, M. Pospíšil<sup>3</sup>, E. Scholtzová<sup>4</sup>**

<sup>1</sup> Department of Environment, Ionian University, 29100, Zakynthos, Greece

<sup>2</sup> Centre for Research and Technology Hellas (CERTH), 15125, Marousi, Greece

<sup>3</sup> Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16, Prague, Czech Republic

<sup>4</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

\* e.gianni@ionio.gr

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**KEYWORDS:** Halloysite | Diclofenac | Drug delivery | Decontamination

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Halloysite (HNT) is a clay mineral of the kaolinite group, extensively known for its unique spiral-shaped nanotubular morphology. Due to its physicochemical features and especially its charge distribution, it is widely used for its interaction with a variety of substances covering a range of applications, including pharmaceutical and environmental uses [1].

Diclofenac is a commercial, non-steroidal, anti-inflammatory analgesic mainly used for pain and inflammation treatment [2]. Its effective loading on halloysite mineral at the targeted drug delivery into the human body is known. However, the mechanisms behind the loading process are still not known in detail.

In the framework of the present study, two forms of diclofenac (D), the neutral ( $D^0$ ) and the anionic one ( $D^-$ ), were examined to investigate the mutual interactions existing between them and the halloysite mineral. The sorption mechanism was explained using classical molecular simulation methods and especially Forcefield (FF) calculations.

The geometry optimization of HNT- $D^0$  and HNT- $D^-$  complexes and the molecular dynamics performed showed a preference for the mineral to attract the neutral form of the active substance. Both forms had the tendency to interact with the alumina octahedral sheet ( $Al(OH)_3$  unit) of halloysite, while the mechanism acted among the initial components (i.e. HNT and D) based on the presence of electrostatic interactions. Strong interactions were observed between the chlorine atoms of D and the halloysite sheets.

Based on the high stability of HNT-D complexes, the halloysite could be used as a potential material for the sorption of diclofenac molecules not only for pharmaceutical applications such as drug delivery, but also as a sorbent for the decontamination of soils or wastewater that are enriched in such contaminant.

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# CHITOSAN-BASED BIONANOCOMPOSITES WITH LAPONITE IMMOBILIZED SILVER NANOPARTICLES FOR DELIVERY OF SUNITINIB MALEATE TO BREAST CANCERS

**P. Labib<sup>1</sup>, G.R. Mahdavinia<sup>2</sup>, A. Akbari<sup>3</sup>**

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36 Bratislava, Slovakia

<sup>2</sup> Polymer Research Laboratory, Department of Chemistry, Faculty of Science, University of Maragheh, 55181-83111, Maragheh, Iran

<sup>3</sup> Solid Tumor Research Center, Cellular and Molecular Medicine Research Institute, Urmia University of Medical Sciences, Urmia, Iran

\* uachshot@savba.sk

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**KEYWORDS:** Chitosan | Laponite | Drug delivery | Antibacterial

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In cancer treatment, multi-drug resistance (MDR) in cancer cells and bacteria is a major challenge that reduces the effectiveness of traditional drug delivery systems (DDSs) [1]. Chemotherapy often weakens patients' immune systems, making them more prone to infections. Over time, both cancer cells and bacteria develop resistance to common drugs, making treatment harder [2]. To address this, we need new drug delivery systems that combine anticancer and antibacterial properties. In the past two decades, nanotechnology and polymer chemistry have created opportunities to develop advanced materials for medicine. Biopolymers, which are biodegradable, biocompatible, and non-toxic, are particularly useful in drug delivery. They are used in various applications, such as binders in capsules, coatings in tablets, and carriers of active ingredients. Chitosan (CTS) is a biopolymer with excellent properties for biomedical use. Adding nanoparticles to CTS can improve its ability to control and sustain drug release. Laponite Rapid Dispersion (Lap RD) is a biocompatible clay that, when combined with CTS, helps control drug release and protect drugs from degradation [3]. In this study, we developed novel pH-sensitive and antibacterial drug carrier systems based on silver nanoparticles (AgNPs) embedded within the interlayers of laponite (Lap) in the presence of chitosan (CTS) for the controlled release of sunitinib maleate (STM). Initially, silver ions and sunitinib maleate were loaded into Lap, and subsequently, a CTS-based hybrid bionanocomposite carrier (Lap@CTS@AgNPs@STM) was synthesized using citric acid as a cross-linking agent. The successful fabrication of the nanocarrier and the formation of AgNPs were confirmed using various analytical techniques, including FTIR, XRD, TGA, SEM, and TEM. TEM images demonstrated the uniform distribution of AgNPs within the Lap@CTS@AgNPs structure. The prepared samples exhibited pH-sensitive anticancer drug release behavior. The release mechanism of STM was analyzed using the Korsmeyer-Peppas and Higuchi kinetic models. Additionally, in-vitro cytotoxicity and antibacterial tests were conducted against the bacteria *S. aureus* and *E. coli*, as well as the MCF-7 cancer cell line, to demonstrate the efficacy of the synthesized samples as multifunctional carrier systems for biomedical applications.

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# THERMALLY TREATED Palygorskite for Table Olive Wastewater Treatment

**C.V. Lazaratou<sup>1,2\*</sup>, D.V. Vayenas<sup>1,2</sup>**

<sup>1</sup> Institute of Chemical Engineering Sciences, Foundation for Research and Technology, PO Box 1414, GR - 26504, Patras, Greece

<sup>2</sup> Department of Chemical Engineering, University of Patras, GR-26504, Patras, Greece

\*c.lazaratou@ac.upatras.gr

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**KEYWORDS:** Adsorption | Clay mineral | Phenols recovery

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The table olive and olive oil production industry is an important contributor to the Mediterranean and EU economy, accounting for 31% of the world's total olive oil production, with Spain and Greece being the main producers [1]. The edible olive processing stages (e.g., pressing, fermentation, packaging) and the residual brine result in large quantities of waste products, which are rich in organic acids and phenolic compounds, and are also characterised by high salinity [2]. Among the many methods being studied, adsorption is considered the best and most affordable technology for the treatment and recovery of phenolic compounds from olive processing waste [3].

In the present work, the treatment of brine and table olive processing waste from a local Greek company, using palygorskite from Geohellas S.A. as adsorbent, was investigated in continuous and batch experiments. Initially, laboratory-scale non-continuous flow experiments were carried out, where the optimal conditions for the removal of organic load (COD), colour and phenolic compounds were determined, examining the effect of adsorbent mass and pH of the wastewater.

Of the ratios tested, 10 g/L adsorbent appeared to be the most effective for the treatment of both the waste and brine, as 60-70% COD and phenolic compound removal was achieved in both cases, while complete decolorization of the waste and brine by 85% was observed. The pH did not appear to affect the process significantly, however at pH values of 2-4 an increased yield of 12% was observed. This was followed by continuous flow experiments in columns until saturation of the palygorskite was reached, in order to approximate the process in a pilot application, and to allow the recovery of phenolic compounds to follow. The results are particularly encouraging for further study of this process, utilizing Greek mineral raw materials for the treatment of a very important waste category for the Greek region, and for the recovery of phenolic compounds useful in a variety of industrial applications using an economical and environmentally friendly adsorbent.

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# ENHANCED PHOTOFUNCTIONAL PROPERTIES OF HYBRID SYSTEMS COMPOSED OF BENZOTHAZOLE-BASED DYES AND LAYERED SILICATES

V. Planetová<sup>1\*</sup>, P. Boháč<sup>1</sup>, J. Bujdák<sup>1,2</sup>

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, 845 36, Bratislava, Slovakia

<sup>2</sup> Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, 842 15, Bratislava, Slovakia

\* viktoria.planetova@savba.sk

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**KEYWORDS:** Benzothiazole Derivatives | Layered Silicates | Spectral Properties | Surface-Fixation Induced Emission

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Photofunctional organic-inorganic hybrid systems form numerous promising materials with tunable optical properties [1]. This study investigates the luminescence enhancement of organic dye molecules adsorbed on layered silicate particles, attributed to surface-fixation-induced emission and aggregation-induced emission. Both phenomena are primarily due to the suppression of non-radiative deactivation via molecular motion [2].

This work focuses on the preparation of hybrid materials composed of novel benzothiazole-based dyes and layered silicate nanoparticles with the main objective of improving photoactivity. We have prepared dispersions of two cationic dyes: 2-(4-(diphenylamino)styryl)-3-methylbenzothiazole-3-ium iodide (SIG373) and 2,6-bis(4-(diphenylamino)styryl)-3,7-dimethylbenzobis(thiazole)-3,7-dium iodide (AC111) with synthetic saponite (Sap) in ten different  $n_{\text{dye}}/m_{\text{Sap}}$  ratios. The photophysical properties of the pure AC111 and SIG373 dye solutions and the hybrid dye dispersions with Sap were compared using spectroscopic methods, such as UV-VIS spectroscopy, fluorescence spectroscopy, time-resolved fluorescence spectroscopy, and quantum yield measurements.

By adsorption on Sap particles, we were able to stabilize the dyes against changes in absorbance (bleaching), which occurred to a high degree in pure solutions of SIG373. Hybrid dye/Sap systems demonstrated substantial emission enhancement compared to dye solutions, with the emission intensity dependent on the dye/Sap ratio. Two significant trends in fluorescence behavior were observed: an enhancement in emission intensity over time (after 24 h and 7 days) and an exponential decrease in intensity with an increasing  $n_{\text{dye}}/m_{\text{Sap}}$  ratio.

The most photochemically efficient system was obtained at a ratio of 0.01 mmol/g after 7 days, with fluorescence quantum yields of 1.91% and 3.13% for AC111/Sap and SIG373/Sap, respectively. These results emphasize the potential of dye/Sap hybrid systems for advanced photochemical applications.

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## POSTER PRESENTATIONS



# ADSORPTION-INDUCED EMISSION IN HYBRID SYSTEMS OF PORPHYRINS AND LAYERED SILICATES

P. Boháč<sup>1</sup>, R. Sasai<sup>2</sup>, T. Fujimura<sup>2</sup>, V. Planetová<sup>1</sup>, J. Bujdák<sup>1,3</sup>

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

<sup>2</sup> Graduate School of Natural Science and Technology, Shimane University, 1060, Nishi-Kawatsu-Cho, Matsue 690-8504, Japan

<sup>3</sup> Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15, Bratislava, Slovakia

\* [peter.bohac@savba.sk](mailto:peter.bohac@savba.sk)

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**KEYWORDS:** Adsorption-induced emission | Metalloporphyrins | Synthetic saponite |

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The ability of metalloporphyrins to sensitize highly reactive singlet oxygen is a useful tool with potential applications in synthetic photochemistry and environmental and medical fields, such as antibacterial materials. However, for many of these applications, it is necessary to immobilize the photosensitizers on solid carriers, which can pose a challenge due to molecular aggregation of the dye molecules, leading to reduced photophysical properties of the dyes and, therefore, reduced singlet oxygen production as well [1].

This study investigates the relationship between the interactions of two metallo-porphyrin-based photosensitizers with synthetic saponite Sumecton SA and the photophysical properties of final hybrid systems. We studied different systems of porphyrins by varying the silicate/dye ratio ( $n_{\text{dye}}/m_{\text{silicate}}$  - mmol/g). At low silicate/dye ratios, we observed a significant increase in the fluorescence of both photosensitizers. This phenomenon can be explained using the phenomenon of adsorption-induced emission [2]. Adsorption-induced emission is caused by the planarization of metalloporphyrins on the smectite surface. This planarization suppressed the non-radiative deactivation of molecules, leading to a significant fluorescence increase [3]. As the silicate/dye ratio increases, the effect of adsorption-induced emission decreases, while there is also a change in the ratio of the two spectral components identified by MCR analysis.

Overall, these findings provide insights into optimizing photophysical properties in photosensitizer immobilization on solid carriers, which could have significant implications for the development of new applications in various fields, especially in ROS photosensitization

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# UTILIZATION OF INFRARED SPECTROSCOPY FOR THE STUDY OF HYBRID SYSTEMS BASED ON SMECTITE AND QUATERNIZED CHITOSAN PREPARED BY LBL METHOD

V. Kureková<sup>1\*</sup>, D. Kováčik<sup>2,3</sup>, M. Pribus<sup>1</sup>

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

<sup>2</sup> Department of Experimental Physics, Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava, 842 48, Bratislava, Slovakia

<sup>3</sup> CEPLANT, Department of Physical Electronics, Faculty of Science, Masaryk University, 611 37, Brno, Czech Republic

\* [valeria.kurekova@savba.sk](mailto:valeria.kurekova@savba.sk)

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**KEYWORDS:** Trimethyl chitosan | Smectite | Layer-by-layer | Infrared spectroscopy

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Chitosan (CH) is widely known as antibacterial, biocompatible and biodegradable polymer. After quaternization of CH, its use is expanded not only due to increased solubility in water but also increased antibacterial activity. Quaternized CH - N,N,N-trimethyl chitosan (TMCH) and two smectites with different cation exchange capacity (CEC) were used for preparation of hybrid systems by layer-by-layer (LBL) method. The objective of the work was to study the influence of the smectite layer charge on the resulting properties of hybrid systems with using of infrared spectroscopy (IR). TMCH was prepared by two-stage quaternization reaction of CH and iodomethane. The success of reaction was controlled by H-NMR and IR spectroscopy in the middle and near IR region. For preparation of hybrid films smectites Sumecton (S; CEC = 0.72 mmol/g) and montmorillonite Lutilla from new Slovak deposit (L; CEC = 1.04 mmol/g) were used. The polypropylene glass (PP), used as substrate for LBL films, was activated by DCSBD plasma for 20 s at ambient air and dived to TMCH, resp. CH solution. After the activation the PP was dived to stock solutions of S, resp. Lu and again CH, resp. TMCH and it was marked as the first layer of LBL film. Films were prepared by alternating layers of cationic CH and TMCH molecules and negatively charged S and Lu until reaching of 20 layers of LBL film. The infrared spectra were measured by ATR method after every layer and the most intensive changes were observed in the 950 – 1100 cm<sup>-1</sup> region caused by Si-O stretching vibration bands of smectites and C-O stretching vibration of CH, resp. TMCH. With increasing number of layers, the region increased in order: CH-S<TMCH-S<CH-Lu<TMCH-Lu and showed the thickest film was prepared from Lu with higher CEC than from S and TMCH created thickest films with comparison of CH. On the prepared samples was tested also stability of LBL films in water. The samples (20 layers) were deep into water and shaken for 1 hr and 24 hrs. After this the samples were again measured by IR spectroscopy and region from 950 to 1100 cm<sup>-1</sup> was analysed. After 1 hr of deeping the most intense decrease of the peak area was observed for TMCH-Lu (13.9%) and least significant for CH-S (0.6%), after 24 hrs the most intense decrease was observed for CH-Lu (28.8%) and least significant for TMCH-S (8.9%). IR spectroscopy revealed influence the type of used smectite not only for the thickness of LBL films but also for the stability in water.

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# APPLICATION OF INFRARED TECHNIQUES IN CLAY MINERALS INVESTIGATIONS

J. Madejová<sup>1\*</sup>

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

\*[jana.madejova@savba.sk](mailto:jana.madejova@savba.sk)

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**KEYWORDS:** IR spectroscopy | Transmission | Reflection

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Infrared (IR) spectroscopy is frequently used to investigate the structure, bonding and chemical properties of clay minerals. Various sampling techniques (transmission and reflection) are utilized in the clay mineral studies; the choice of the method depends on the task to be solved and on the physical state of the sample. KBr pressed disk technique, the most frequently used transmission method in the middle IR (MIR) region, has been found to be very useful for a routine characterization of clay minerals. The sensitivity of the OH stretching vibrations to structural features of the individual clay minerals permits to differentiate 1:1 vs. 2:1 silicate layer type and to recognize the type (di- or tri-octahedral) and chemical composition of the octahedral sheets. Structural modification of the minerals during various chemical treatments is often studied by KBr technique. Transmission measurements of self-supporting films within a heated cell allow *in situ* study of smectite dehydration. Reflection techniques have been used for samples, which are difficult to analyze by transmission methods or when investigation of a specific problem requires special handling. Attenuated total reflection (ATR) technique was applied to obtain information on the wet clay samples. The exchangeable cations modify both the position and the intensity of the H-O-H stretching band of water near 3400 cm<sup>-1</sup>. Its position decreases in order K<sup>+</sup>, Na<sup>+</sup>, Ca<sup>2+</sup>, Mg<sup>2+</sup>. Using ATR the presence of smectite in extremely diluted suspensions obtained after centrifugation has been detected. Diffuse reflectance (DRIFT) technique in the MIR region has been successfully utilized for identification of low amount of illite layers containing ammonium. DRIFT is a main method employed in the near IR region because allows obtaining spectra of the neat samples, which simplifies and accelerates the IR measurements. The OH overtone region provides useful information about changes in the clay minerals structure upon heating or acid treatment.

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# COMPOSITE MATERIALS BASED ON MONTMORILLONITE MODIFIED WITH CATIONIC AND NON-IONIC POLYMERS

J. Madejová<sup>1\*</sup>, M. Barlog<sup>1</sup>, M. Slaný<sup>1</sup>, Ľ. Jankovič<sup>1</sup>

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

\*jana.madejova@savba.sk

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**KEYWORDS:** Poly(ethylenimine) | Poly(methyloxazoline) | Intercalation |

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The effect of various loadings of cationic poly(ethylenimine) (PEI) and non-ionic poly(2-methyl-2-oxazoline) (PMeOx) into Na-montmorillonite (Mnt) on the physico-chemical characteristics of composites was investigated using XRD, TG/DTG and IR spectroscopy. For PEI-Mnt, almost complete exchange of Na<sup>+</sup> with PEI cations was found, implying that the PEI chains interacted with the Mnt interlayer surface electrostatically. In PMeOx-Mnt, the content of Na<sup>+</sup> remained the same as in Na-Mt, indicating that PMeOx chains are adhered to the Mt surface by hydrogen bonds and/or van der Waals forces. The XRD patterns of PEI-Mnt showed gradual increase of the  $d_{001}$  value from 1.25 nm (Na-Mnt) up to 1.38 nm for sample with PEI concentration corresponding to ~100% CEC of Na-Mt. No change in the basal spacing was observed for the samples prepared with higher cationic polymer loadings. In contrast, a stepwise expansion of the interlayer space of Mnt up to 2.06 nm with increasing amount of non-ionic PMeOx revealed unexpected and very high adsorption of PMeOx on Mnt interlayers. The carbon, TG/DTG and IR analysis, however, indicated a gradually increasing content not only for PMeOx but also for PEI in the samples prepared with higher polymers loadings. It is evident, that at high loadings some of the polymer chains were adsorbed on the Mnt outer surface. The obtained results widen the knowledge on the interactions between polymer and montmorillonite essential for designing novel composites for environmental and/or industrial applications.

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# CONFINEMENT-INDUCED SPECTRAL CHANGES OF DICATIONIC NAPHTHALENE DERIVATIVE

**M. Matejdes<sup>1\*</sup>, J. Bujdák<sup>1,2</sup>**

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

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

\*[marian.matejdes@savba.sk](mailto:marian.matejdes@savba.sk)

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**KEYWORDS:** Synthetic saponite | Naphthalene | Singular value decomposition | Parallel factor analysis

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The confinement of organic cationic dyes within the interlayer space of layered silicates often induces spectral changes that differ from their behavior in pure solvents.[1] Therefore, interlayer space provides an intriguing microenvironment that enables some control over the optical properties of the intercalated organic molecules. However, the spectral changes induced by confinement are not always fully understood, and a comprehensive analysis of the observed changes is lacking, which could lead to a better understanding of the underlying processes. In this study, we focus on the confinement-induced spectral changes of 4,4'-(2,6-naphthalenediyl)dipyridine dications within the interlayer space of synthetic saponite. Varying the exchanged amount of organic dications results in the presence of different species with distinct optical properties. Properties such as emission color and quantum yield strongly correlated with the relative amounts of the present species. To understand how the exchanged amount relates to the presence of different species, UV-Vis spectra and excitation-emission matrices of thin hybrid films were analyzed by using statistical methods such as singular value decomposition and parallel factor analysis.

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# THE ADSORPTION OF Pb(II), Ni(II) AND Cu(II) FROM AQUEOUS SOLUTION BY NATURAL BENTONITE

Z. Melichová<sup>1\*</sup>, M. Šuránek<sup>1</sup>

<sup>1</sup> Department of Chemistry, Faculty of Natural Sciences, Matej Bel University in Banská Bystrica, Tajovského 40, 974 01, Banská Bystrica, Slovakia

\*zuzana.melichova@umb.sk

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**KEYWORDS:** Bentonite clay | Adsorption | Metals | Langmuir isotherm

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Local bentonite clay from the Lieskovec deposit (central Slovakia) was characterized and tested for its ability to adsorb Pb(II), Ni(II) and Cu(II) ions from aqueous solutions. The clay material was characterized using X-ray diffractometry (XRD), Diffuse Reflectance Infrared Fourier Transform (DRIFT) analysis, and Scanning Electron Microscopy (SEM) with Energy Dispersive Spectroscopy (EDS). The main mineral in the bentonite clay was iron-rich montmorillonite, and admixtures such as kaolinite, quartz, cristobalite and plagioclase. In the past, in addition to mineralogical properties [1], geotechnical properties and permeability of bentonite samples from the Lieskovec deposit were also studied [2].

All adsorption experiments were performed at room temperature. The experiments were carried out under batch process with the initial concentration Pb(II), Ni(II) and Cu(II) ions, the amount of bentonite clay, pH, and time as the variables. In addition, the bentonite clay was tested for the adsorption of metal ions without preliminary treatment. A flame atomic absorption spectrometer was used for measuring the metal concentration before and after adsorption [3-4].

Adsorption was very fast at low coverage and equilibrium was approached within 30 min. It was found that the amount of adsorption of metal ion increased with increasing initial pH of the solution, metal ion concentration and contact time, but was decreased with the amount of adsorbent.

Several isotherm models were used to describe the experimental data and to obtain the constant parameters. It was found that Langmuir isotherm model correlated well with the experimental data. The Langmuir maximum adsorption capacity of the Pb(II), Cu(II) and Ni(II) ions was found to be 48.1; 12.24 and 11.34 mg/g, respectively. The results best fitted the pseudosecond-order kinetic model, with the rate constant in the range of  $3.9 \times 10^{-2} - 8.4$  g/mg min.

The study suggests that bentonite clay from Lieskovec can be efficiently used as an inexpensive material for heavy metal ions elimination, mainly for the removal of Pb(II) ions.

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# COMPARISON OF ADSORPTION EFFECTIVITY OF LAYERED INORGANIC STRUCTURES FOR BENZETHONIUM CATION BY DFT METHOD

E. Scholtzová\*

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 84536, Bratislava, Slovakia

\* e-mail [eva.scholtzova@savba.sk](mailto:eva.scholtzova@savba.sk)

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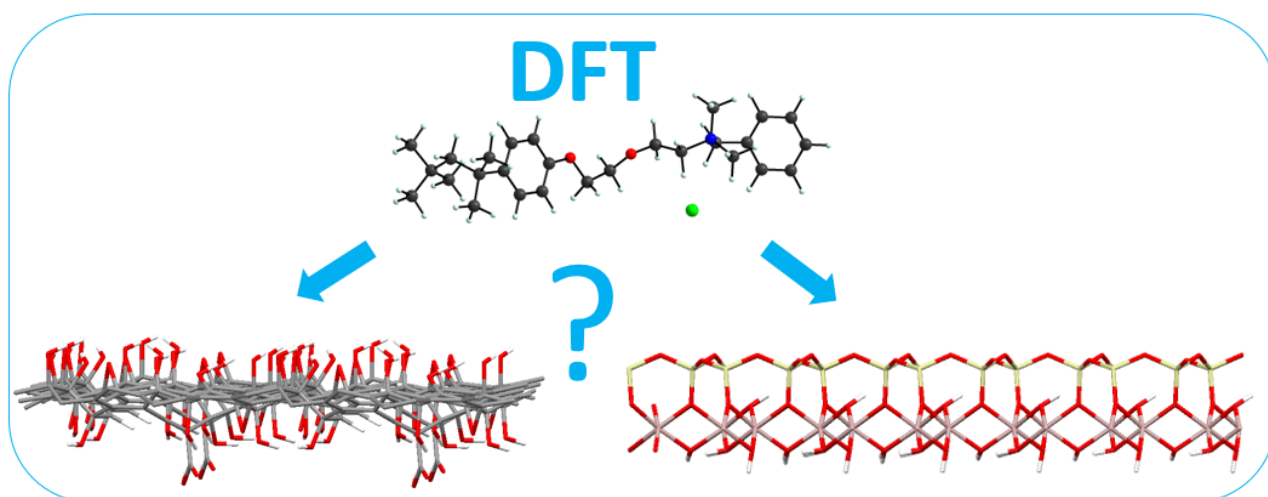
**KEYWORDS:** Benzethonium chloride | Kaolinite | graphene oxide | DFT-D3

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Benzethonium chloride (BtCl) is a synthetic quaternary ammonium salt with antiseptic and anti-infective properties used, e.g., as a topical antimicrobial agent in first-aid antiseptics. Due to its extensive use, we can find this salt in the wastewater. Thus effective sorbent material for the immobilization of BtCl is appreciated. This work studies the effectivity of two layered structures, kaolinite and graphene oxide (GO) as possible sorbent materials of BtCl by the density functional theory method (DFT) with the Tkatchenko-Scheffler (TS) scheme for dispersion.

Kaolinite (K) is a clay mineral widely used in the technological processes. Its big advantage is price, which is much lower than for another effective sorbent, GO.

Both materials have two different surfaces and this study aims to compare the adsorption effectivity and stability of both hybrid systems, BtCl-K and BtCl-GO.



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# INFRARED SPECTRA OF FUNCTIONAL SURFACES BASED ON ORGANO MODIFIED SAPONITE-PHLOXINE COMPOSITE DEPOSITED ON POLYMERS

E. Skoura<sup>1</sup>, H. Pálková<sup>1\*</sup>, J. Bujdák<sup>1,2</sup>, S. Zimowski<sup>3</sup>

<sup>1</sup>. Institute of Inorganic Chemistry SAS, Dúbravská cesta 9, 845 36 Bratislava, Slovakia

<sup>2</sup>. Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, Bratislava, Slovakia

<sup>3</sup>. Faculty of Mechanical Engineering and Robotics, AGH University of Krakow, al. A. Mickiewicza 30, 30-059 Krakow, Poland

\* [helena.palkova@savba.sk](mailto:helena.palkova@savba.sk)

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A thin nanocomposite layer composed of organoclay and the fluorescent dye phloxine B (PhB) was deposited on the polymer matrix to prepare luminescent and antibacterial material [1]. The principle was the fusion of a thin layer of organoclay composite with a polymer matrix poly(caprolactone) (PCL) to design materials with a surface available for further reactions. The surface profile of the polymer pellets was examined via optical profilometry to measure the roughness and topography of the surface. Results showed an increase in the surface roughness after the surface modification from 46 to 162 nm. The predominance of the polymer matrix, smectites, and organic species within the studied system could be challenging for the identification of minor constituents in similar systems. Infrared (IR) spectroscopy was used to characterize such materials, detect and identify individual components. Single components, i.e., Sap, DDOA (dioctadecyldimethylammonium), PhB, and PCL, were also analyzed to reveal distinct bands needed for their identification. IR spectroscopy was employed to investigate the functional groups present on the surface of various samples, including single components such as Sap, DDOA, PhB, and PCL. Sap exhibited bands at 3678 cm<sup>-1</sup>, 980 cm<sup>-1</sup>, 658 cm<sup>-1</sup>, and 467 cm<sup>-1</sup>, corresponding to Si–O and structural O–H vibrations. The bands at 2917 cm<sup>-1</sup>, 2850 cm<sup>-1</sup>, and 1466 cm<sup>-1</sup>, attributed to the C–H vibrations of DDOA cations, emerged in the organo-modified sample spectrum. PhB showed characteristic bands in the fingerprint region, with a detectable weak band at 1357 cm<sup>-1</sup> for aromatic C–C bending vibrations. Additional small bands near 1557 cm<sup>-1</sup> and 1237 cm<sup>-1</sup> indicated the presence of dye molecules. PCL was identifiable by a sharp band at 1725 cm<sup>-1</sup> for C=O stretching vibrations and a band at 1177 cm<sup>-1</sup> for C–O–C bonds. These bands were also present in the spectra of composites with organoclays, PCL\_OC, and PCL\_PhB0.1. Despite the low dye content and overlapping bands from dominant phases, a small band at 1560 cm<sup>-1</sup> confirmed the incorporation of dye in the PCL\_PhB0.1 sample. In this context, infrared spectroscopy emerged as a valuable tool for characterization.

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# PHYSICOCHEMICAL ASPECTS AND HYDRATION PROPERTIES OF POLY(2-ETHYL-2-OXAZOLINE) AND POLY(DIALLYLDIMETHYLAMMONIUM CHLORIDE) FUNCTIONALIZED MONTMORILLONITE

**M. Slaný<sup>1,2\*</sup>, Ľ. Jankovič<sup>1</sup>, M. Matejdes<sup>1</sup>, J. Madejová<sup>1</sup>**

<sup>1</sup> Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

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

\*[michal.slany@savba.sk](mailto:michal.slany@savba.sk)

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**KEYWORDS:** Montmorillonite | Poly(2-ethyl-2-oxazoline) | Poly(diallyldimethylammonium) | Hydration

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The novel functionalized montmorillonites (Mts) with non-ionic poly(2-ethyl-2-oxazoline) (PEtOx) and cationic poly(diallyldimethylammonium) (PDDA) were created via an intercalation method with different loading ratio of both polymers. Their comprehensive physicochemical characteristics were analysed through carbon analysis, PXRD, FTIR, TGA/DSC and BET-N<sub>2</sub> adsorption analysis. The influence of hydration on PEtOx-Mts and PDDA-Mts was investigated using gravimetric analysis and NIR spectroscopy. PXRD analysis showed a significant increase in 001 diffraction of PDDA-Mt corresponding to a PDDA interlayer with a  $d_{001}$  ranging from 1.47 to 1.49 nm. Conversely, the basal spacing exceeding 2 nm for PEtOx suggested, that the PEtOx polymer was intercalated in a larger amount and packed in a less compact manner compared to PDDA. After modification of Na-Mt with PEtOx polymer, FTIR spectroscopy revealed the presence of the carbonyl C=O group (3265 and 1641 cm<sup>-1</sup>) and the stretching (2982, 2942 and 2883 cm<sup>-1</sup>) and bending (1480-1200 cm<sup>-1</sup>) vibrations of the CH<sub>2</sub> and CH<sub>3</sub> groups [1]. The vibrations of the CH groups were also confirmed after PDDA modification. NIR spectroscopy confirmed the vibrational modes assigned to both PEtOx and PDDA polymers. The results of BET-N<sub>2</sub> adsorption analysis showed a significant decrease in the specific surface (SSA) area after modification with a non-ionic PEtOx polymer. On the contrary, in the case of modification of Na-Mt with polycation PDDA, SSA increased slightly in two instances. TG analysis revealed greater mass loss for PEtOx-Mts compared to PDDA-Mts. DTG analysis confirmed the release of physisorbed bound water around 100°C, decomposition of the organic phase within the 250-550°C range and dehydroxylation of OH groups around 550-800°C in both cases. The results obtained from the gravimetry and NIR analysis indicated a greater hydrophobic nature for PEtOx-Mts compared to PDDA-Mts. These findings have considerable potential to improving the properties of novel organo-montmorillonites, thereby facilitating their application as adsorbents for pollutants, biodegradable materials, surface coatings, drug carriers, fillers in polymer nanocomposites, anticancer agents and various other important applications.

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# ADSORPTION OF HEXAVALENT CHROMIUM BY PENTAMER UNIT OF POLY-(N-BUTYL ETHYLENEIMINE)-MODIFIED MONTMORILLONITE

P. Škorňa<sup>1\*</sup>, L. Jankovič<sup>1</sup>, E. Scholtzová<sup>1</sup>, D. Tunega<sup>2</sup>

<sup>1</sup> Institute of Inorganic chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36, Bratislava, Slovakia

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

\*[peter.skorna@savba.sk](mailto:peter.skorna@savba.sk)

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**KEYWORDS:** Montmorillonite | DFT-D3 | Chromate pollutant |

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Compounds based on hexavalent chromium (CrVI), mainly dehydrated or hydrated salts such as Na<sub>2</sub>CrO<sub>4</sub> or Na<sub>2</sub>CrO<sub>4</sub>·4H<sub>2</sub>O, are typical raw materials for the chemical industry. They are used, for example, as corrosion inhibitors [1], in textile dyeing processes [2], inks [3], paints [4], leather tanning [5], wood preservatives [6], and in the production of the other chromium compounds [7]. CrVI salts are also used in metallurgy, electroplating, metal finishing or paper production, and nuclear power plant, where many wastewaters containing chromium ions are produced.

This paper presents the study of the adsorption of toxic hexavalent chromium oxyanion into the interlayer space of pentamer unit of poly-(N-butyl ethyleneimine)-modified montmorillonite. The main aim of this research is to provide a comprehensive structural study of the calculated system. The structural stability of individual systems was determined by analysing the strength and number of hydrogen interactions in combination with the calculated intercalation energies. Moreover, the measured FTIR spectra were investigated by means of the vibrational modes obtained from the calculated spectra using the ab initio molecular dynamics (AIMD) approach.

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## LIST OF PARTICIPANTS

1.	BASHIR SANAM	Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
2.	BILSKÁ KATARÍNA	Department of Microbiology and Virology, Faculty of Natural Sciences, Comenius University in Bratislava, Bratislava, Slovakia
3.	BOHÁČ PETER	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
4.	BUDZÁK ŠIMON	Department of Chemistry, Faculty of Natural Sciences, Matej Bel University, Banská Bystrica, Slovakia
5.	BUJDÁK JURAJ	Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Bratislava, Slovakia
6.	BUJDÁKOVÁ HELENA	Department of Microbiology and Virology, Faculty of Natural Sciences, Comenius University in Bratislava, Bratislava, Slovakia
7.	GEORGE VINNY	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
8.	GIANNI ELENI	Department of Environment, Ionian University, Zakynthos, Greece
9.	KUREKOVÁ VALÉRIA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
10.	LABIB SHOTORBAN PARISA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
11.	LAZARATOU CHRISTINA VASILIKI	Institute of Chemical Engineering Sciences, Foundation for Research and Technology, Patras, Greece
12.	MADEJ JÁN	
13.	MADEJOVÁ JANA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
14.	MATEJDES MARIÁN	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
15.	MELICHOVÁ ZUZANA	Department of Chemistry, Faculty of Natural Sciences, Matej Bel University in Banská Bystrica, Slovakia
16.	PÁLKOVÁ HELENA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava
17.	PLANETOVÁ VIKTÓRIA	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava
18.	SCHOLTZOVÁ EVA	Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava
19.	SLANÁ MARICA	Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava
20.	SLANÝ MICHAL	Department of Hydrosilicates, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava
21.	ŠKORŇA PETER	Department of Theoretical Chemistry, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava





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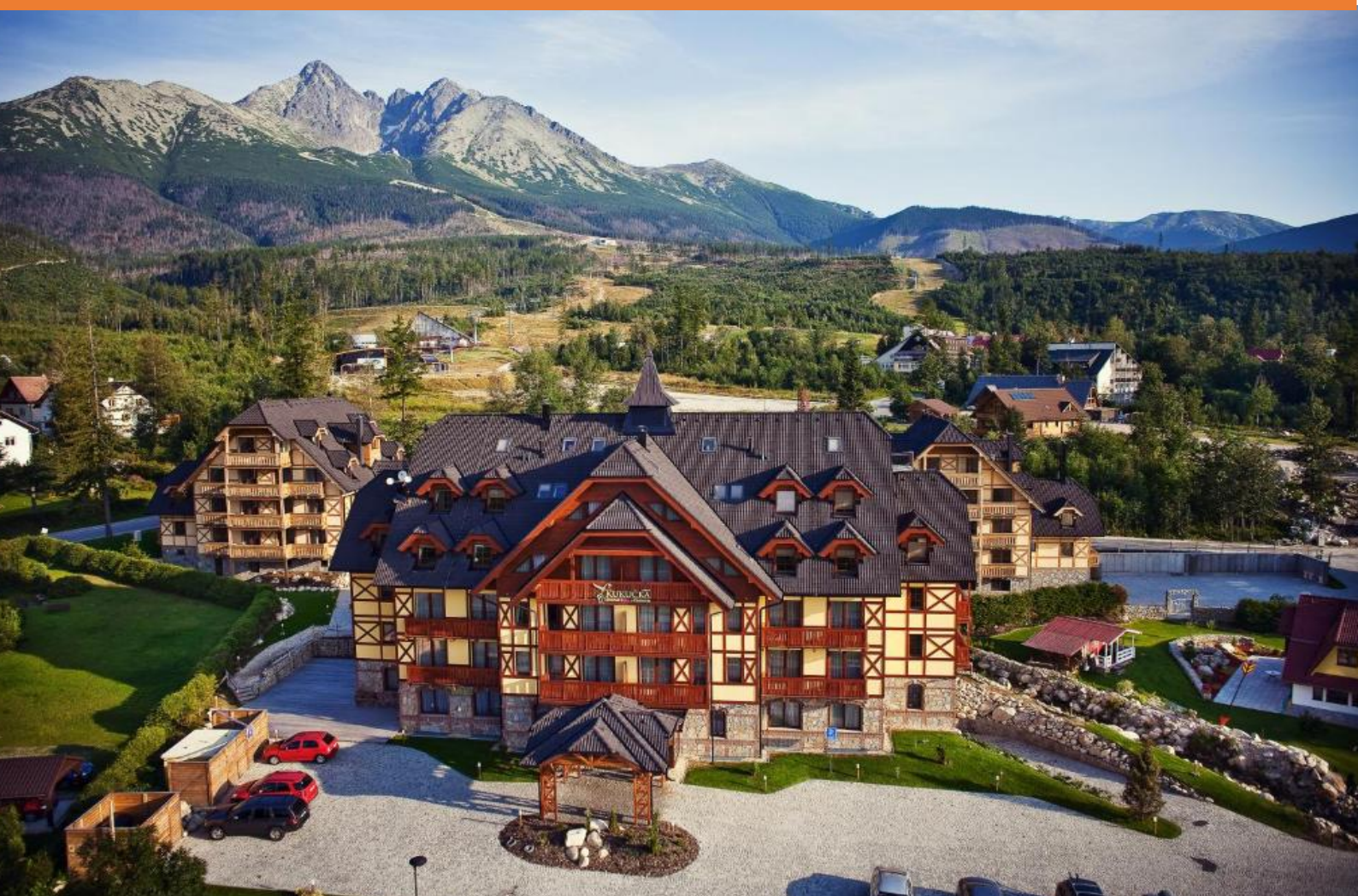
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