



16th Students' Congress of Society of Chemists and Technologists of Macedonia

Book of Abstracts

27-28 October 2025
Skopje, N. Macedonia





Сојуз на хемичарите и технолозите на
Македонија

Society of Chemists and Technologists of
Macedonia

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Society of Chemists and Technologists of Macedonia

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Dear students, esteemed colleagues, and distinguished guests,

It is my great honor and privilege to extend to you all a most cordial welcome to the 16th Students' Congress of the Society of Chemists and Technologists of Macedonia. This year's congress marks 31 years since the very first student meeting organized under the auspices of our Society—an enduring tradition that continues to encourage and celebrate the scientific curiosity and dedication of young researchers.

First, I would like to express my sincere appreciation to all student participants. For many of you, this is your first experience presenting at a scientific conference—and I truly believe it will serve as excellent preparation for larger international events you will attend in the future. This year's program includes 49 student oral presentations, with participants from Macedonia, as well as from Serbia, Bulgaria, Kosovo, Croatia, Turkey, Poland, and Azerbaijan.

We are also honored to host two plenary and five invited lectures, delivered by distinguished colleagues from the Faculty of Technology and Metallurgy and the Institute of Chemistry, both from the Ss. Cyril and Methodius University in Skopje. Among our invited guests are also representatives from the University of Opole in Poland, the Faculty of Agriculture, Goce Delčev University in Štip, and the pharmaceutical company Alkaloid AD Skopje.

I'd like to take a moment to sincerely thank the organizers of this event, Iva Dimitrievska and Marija Proševa, for their amazing dedication and organizational talent. Thanks to their hard work and enthusiasm, this event has come to life—and we're all able to share this wonderful experience together.

During the pandemic, we had to adapt to communicating solely online—and while that worked under the circumstances, it also reminded us how much we value real, face-to-face links. Even though online conferences still have their benefits, nothing can truly replace the energy and inspiration that come from being together in person.

Dear students, I encourage you to make the most of this wonderful opportunity—to share your chemistry achievements, celebrate your hard work, and exchange ideas with one another. This meeting is not just about presenting results; it's about finding inspiration, forming collaborations, and creating lasting friendships. Most importantly, it's about building genuine personal chemistry.

I wish you all successful presentations and an enjoyable and inspiring stay. May this meeting be a memorable step in your scientific journeys, and I look forward to welcoming you again at our future events.

Prof. Zoran Zdravkovski, president

Society of Chemists and Technologists of Macedonia



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***PLENARY AND
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PL – 1

Polymer based composites

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Polymer based composites obtained by IR laser-induced ablation is attracting particular attention due to the specific application of the resulting thin films. This technique is promising in terms of the fabrication of polymers containing polar groups that can serve as protective layers to different nano-bodies, metals, metal chalcogenide's and conductive polymer nanocomposites. We have examined IR laser-induced ablative deposition with polyvinyls loaded with Fe and Cu particles to establish its specific features and differences from conventional pyrolysis.

It was of interest to us to continue our previous effort and we focused on composites from different type of carbon nanofillers incorporated into acrylic/methacrylic matrices. Therefore, graphene nanoribbons, or mixture of graphene/carbon nanotube filler incorporated within polymer matrix, will not only reinforce mechanically and thermally the composite materials, but will significantly expand their application potential, giving added value to the cheap polymeric material.

Polymeric microspheres based on methyl methacrylate, ethylene glycol dimethacrylate, divinylbenzene and *N,N'*-methylenebisacrylamide were applied in our next research for the removal of acidic and basic dyes and phenol from effluents. To address the challenges associated with the effective removal of inorganic and organic impurities by the adsorption technique, new adsorbents in the form of polymer microspheres based on ethylene glycol dimethacrylate and vinyl acetate containing starch modified with boric acid and dodecyl-S-thiuronium have been synthesized and then they were characterized by using the ATR/FT-IR, DSC, EDS, SEM and BET.

Integrating multi-walled carbon nanotubes into and on the surface of polymer matrices, such as nylon, by spray coating or spin coating method has shown promise in creating materials with superior mechanical, electrical, thermal properties and potential use in triboelectric nanogenerators. The multi-walled carbon nanotubes not only improve the dielectric properties but also increase the concentration of charge carriers, facilitating more efficient charge transfer and a higher output. These results are valuable for guiding the design of next generation triboelectric nanogenerators with optimized nanocomposite compositions for wearable electronics, low-power sensing systems, and sustainable energy harvesting technologies.

Keywords: polymer-based nanocomposites, triboelectric nanogenerators.



Minerals of Macedonia: Insights from Vibrational Spectroscopy, Structural and Thermal Studies

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The diversity and distribution of mineral species in our country are exceptionally extensive. Comprehensive mineralogical investigations have identified approximately 145 distinct mineral species occurring within the country. Of these, 100 have been systematically collected, classified, identified, and characterized by our research group. Out of the 6176 mineral species globally approved by the International Mineralogical Association (as of September 2025), twenty were first discovered in N. Macedonia. Among these, seven remain endemic (four oxides, two silicates, and one arsenate), while five mineral species bear toponym-based names honoring geographic features of the country: macedonite, nežilovite, dorallcharite, zincovelesite-6N6S, and babunaite-(Nd).

Over the past twenty-five years, systematic research has been conducted primarily on the vibrational spectroscopic and structural characteristics of Macedonian minerals, resulting in the publication of more than fifty papers in reputable international journals. Several of these studies, focusing on rare and scientifically intriguing minerals have also been adapted into didactic mineralogical and chemistry materials, designed to effectively communicate modern chemical concepts to students through structured and rich illustrated content.

The scientific investigations have addressed a wide range of topics, including the elucidation of photoinduced phenomena in some minerals; determination of accurate chemical compositions in minerals with variable stoichiometry; development of analytical methodologies for the elimination of matrix effects and the detection of rare or trace elements; examination of thermal behavior with emphasis on dehydration processes; comparison of vibrational spectra of natural minerals with their synthetic analogues; identification of mineral associations within complex matrices; interpretation of vibrational spectra variations observed within isomorphic mineral series, etc. Selected results of some of these studies are presented herein.

Keywords: minerals, vibrational spectroscopy, structural features, thermal studies.



Smart Chemistry in Action: Modern Methods and Sustainable Practices in Chemical Synthesis

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Chemical synthesis today is undergoing a transformation, shaped by the need for efficiency, sustainability, and innovation. Traditional stepwise approaches are being complemented, and sometimes replaced by new methodologies that expand the chemist's toolbox. Among these, microwave-assisted synthesis, catalysis, and one-pot or multicomponent reactions stand out as strategies that accelerate discovery while reducing waste and energy consumption. Beyond methodology, this transformation is also driven by the principles of green and sustainable chemistry. Practical actions such as solvent recycling, microwave heating, digitalisation through electronic laboratory notebooks, and the use of energy-efficient laboratory equipment demonstrate how theoretical concepts of green chemistry can be turned into measurable reductions in waste, water, and energy use. These practices represent not only environmental responsibility but also a more resource-efficient and innovative way of conducting chemical research and education. As a case study, the research based on the synthesis and characterisation of pyrene and azapyrene derivatives, explored as structural isosteres with potential in donor–acceptor systems, fluorescent probes, and thermoresponsive materials, will be presented. These examples show how modern synthetic methods, aligned with sustainable practices, not only change how we build molecules but also broaden what kinds of functional materials we can design. The goal of this talk is to inspire young researchers to view synthesis as a creative and evolving discipline, where modern strategies and sustainable practices converge to shape the future of chemistry.

Keywords: Modern synthetic methods, Microwave-assisted synthesis, Green chemistry, Sustainable laboratory, Pyrene, Azapyrene, Donor–acceptor systems, Photophysical properties, Fluorescence, Solvatochromism

Acknowledgment: This research was funded by the National Science Centre, Poland, under the SONATA programme, grant no. 2023/51/D/ST5/00369.



Synthesis and photo-induced properties of TiO₂/ZnAl LDH, TiO₂/Kaolinite and TiO₂/Ielite based photocatalysts

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The aim of this study was to develop photocatalysts based on TiO₂/ZnAl layer double hydroxides (LDHs), TiO₂/Kaolinite and TiO₂/Ielite that can be activated by UV/VIS irradiation. A series of TiO₂/ZnAl LDHs, TiO₂/Kaolinite and TiO₂/Ielite based composites were synthesized, and their self-cleaning and photocatalytic efficiency were tested in the photodegradation of rhodamine B under UV/VIS light irradiation. The influence of TiO₂ doping (3 and 10 w.t. %, impregnated by mechanical activation in planetary and attrition mill) on the photo-induced properties of developed nanocomposites was studied. Suspensions of TiO₂/ZnAl LDHs, TiO₂/Kaolinite and TiO₂/Ielite composites were applied as coatings on three types of substrates: porous, highly porous and non-porous. The different functional behaviors of the coatings were interpreted in correlation with their structural, textural and morphological properties.

The results obtained in this study indicate that the photocatalytic activity of the coatings generally depends on the method of TiO₂ impregnation into the support and the amount of TiO₂ loaded. The findings suggest that using mechanical activation for synthesis resulted in a homogeneous distribution of TiO₂, enhancing the accessibility of active sites within the photocatalytic coating. These novel TiO₂-based coatings present advantages in terms of low cost and simple preparation while ensuring high photodegradation efficiency.

Keywords: photocatalysis, TiO₂, layer double hydroxides, kaolinite, ilite, coatings



LC-ESI-MS/MS characterization of phenolic compounds, selenium species and vitamins in red winemaking

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Red winemaking has a very long tradition in Republic of N. Macedonia. The dominant red variety is Vranec, followed by Merlot, Cabernet Sauvignon and Kratošija. Kratošija is as an old ancient Balkan variety, grown at the Macedonian vineyards in the period when wine was produced in amphora. In the period of Yugoslavia, specifically in the 1950s, Kratošija was replaced with Vranec variety and nowadays, Kratošija is found in a small vineyards alone, and mainly in a combination with the Vranec vines¹. Since there are limited published studies for Kratošija, the aim of this work was application of HPLC-ESI-MS/MS technique for chemical characterization of Kratošija wines, including identification, quantification and semi-quantification of various compounds such as phenolic compounds (flavonoids and nonflavonoids), selenium species and vitamins. Moreover, Kratošija wines were produced by inoculation of two commercial yeasts (ZymafloreTM Xpure (Laffort) and Lalvin ICV D80 (Lallemand)), in order to study the effect of the yeast on the content of the determined compounds. It was noticed that yeast affected the phenolic profile of wines, probably as a result of the different fermentation rates. Thus, flavan-3-ols, antohocyanins monoglycosides and antohocyanins acetylglucosides were present in a higher content in the wine fermented with the Lalvin ICV D80 yeast. Flavones chrysin and luteolin, flavanone naringenin, flavanonol taxifolin, stilbenoid ϵ -viniferin, as well as selenium species (selenomethionine, selenomethionine oxide and selenium methylselenoselenocysteine) and vitamins (panthotenic acid (B5), thiamine (B1) and nicotinic acid (B3)) were reported for the first time in Macedonian red wine.

Keywords: Polyphenols, selenium species, vitamins, yeast fermentation, red winemaking, Kratošija, HPLC-ESI-MS/MS.

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Acknowledgements: This work was supported by the CEEPUS Network (RO-0010) Teaching and Learning Bioanalysis, covering the study stay of Violeta Ivanova-Petropulos at the Department of Chemistry, University of Warsaw, Poland, where she performed the analyses.



Advances in Sensory Evaluation and Oral Perception of Sourdough Gluten-Free Muffins Incorporating Tomato Pomace

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The demand for gluten-free products is growing, with texture considered a crucial factor. This research focuses on developing gluten-free muffins based on rice flour, fermented with sourdough and enriched with 10% tomato by-product. The study examines sensory properties influenced by fermentation duration (0h, 24h, 48h). Sensory acceptability was assessed using both classical hedonic analysis with 58 respondents from North Macedonia and Bulgaria and advanced biometric analysis employing OCOsense™ smart glasses, which monitor facial expressions and chewing behavior. Moreover, the average saliva absorption from the formed boluses of the subjects was calculated as an indirect parameter of palatability and textural comfort.

The sensory analysis of our gluten-free muffins showed generally positive feedback, especially for their appearance and overall impression, from both Macedonian and Bulgarian participants. We found that longer sourdough fermentation (24 to 48 hours) noticeably improved the taste and texture, with Bulgarian tasters giving more consistent and higher scores—likely due to their greater familiarity with fermented baked goods. Using OCOsense™ glasses, we objectively measured chewing behavior and saliva absorption, revealing that longer fermentation reduced how much saliva the muffins absorbed and led to more frequent chewing, which could explain the differences in mouthfeel. We also saw clear differences between generations and cultures, demonstrating how these factors play an important role in how these gluten-free products are perceived and enjoyed.

By combining traditional sensory tests with advanced biometric tools, we gained a complete picture of the muffins' sensory qualities, texture, emotional impact, and how they are processed in the mouth. This innovative approach offers a new way to evaluate functional gluten-free baked goods. Importantly, all our testing followed strict ethical guidelines for sensory research.

Keywords: functional product, by-product valorization, gluten-free, oral processing, sensory perception



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IL – 5

Chemical Engineer in the Pharmaceutical Industry – Becoming a Value-Based Leader

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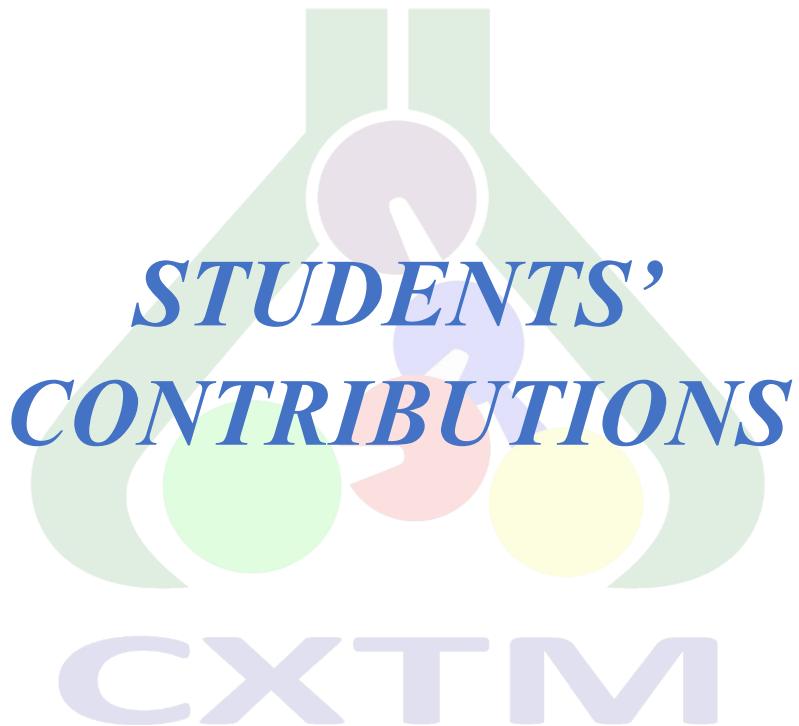
A professional journey begins with the choices made during formal university education. These decisions ideally practical, forward-looking, and supported by an exit strategy lay the foundation for future career development. Equally important are the professional connections built during academic and industry experiences, particularly with individuals who share similar values, ambitions, and aspirations. Beyond education and networking, active engagement with the community strengthens leadership capacity, as contributing positively to society inspires others to do the same.

Value-based leadership integrates personal principles such as integrity, ethics, innovation, accountability, and transparency into one's leadership style. Central to this approach is continuous self-reflection, allowing leaders to evaluate and challenge themselves while remaining aligned with their values¹. Importantly, leadership is not dependent on formal titles; rather, it emerges through consistent actions and influence². In this way, chemical engineers in the pharmaceutical industry can position themselves not only as professionals but as leaders who create lasting value.

Keywords: chemical engineers, pharmaceutical industry, values based leadership

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SP – 1

Nutritional Characterization of Gluten-Free Sourdough Muffins Enriched with Tomato Industry By-Products

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NOT PRESENTED



Authenthication of Raspberry (*Rubus idaeus*) in Fresh and Processed Food Products Using PCR-HRM Analysis

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In recent years, interest in healthy and natural food products has increased, particularly in fresh fruits and their derivatives, which are important sources of bioactive compounds. However, due to the high cost of fruits and the economic incentives of producers, adulteration of fruit-based products is frequently observed. This study aimed to develop and apply DNA-based methods to verify the authenticity of *Rubus idaeus* (red raspberry) and its derived products. DNA was extracted from fresh fruits, dried fruits, and industrially processed products (teas, juices, jams and smoothies). A commercial DNA isolation kit was used, yielding pure and concentrated DNA suitable for PCR (Polymerase Chain Reaction) analysis. Specific primers targeting the ITS1 (Internal Transcribed Spacer 1) region were designed to enable reliable differentiation of raspberry from closely related species (eg. blackberry, strawberry). DNA extracts were subjected to PCR-HRM (High-Resolution Melting) analysis. The method successfully detected raspberry DNA across all sample types, with dried and minimally processed products producing the strongest signal and the clearest melting curves. Juice samples exhibited lower signal intensity and slightly shifted curves due to industrial processing and lower DNA concentration, while dense products with high sugar and additive content (jams and smoothies) generated weaker, less specific curves. Electrophoresis confirmed the specificity of the amplicons, showing a product of approximately 220 bp for raspberry and distinct amplicons for related species. These findings demonstrate the high selectivity, sensitivity, and applicability of PCR-HRM as a reliable tool for fruit product authentication and adulteration detection, with strong potential for routine quality control and consumer protection.

Keywords: *Rubus idaeus*, food authenticity, PCR-HRM, DNA barcoding, electrophoresis

Acknowledgements: We gratefully acknowledge the grant support from University Student Assembly of the „Ss. Cyril and Methodius“ University in Skopje for the project titled „Determining the authenticity of fruit products using PCR methods“.



Optimization of a Method for Analysis of Residual Solvents in Food Packaging Using Headspace Sampling and Gas Chromatography Coupled with Mass Spectrometry (HS-GC-MS)

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Food packaging materials, often composed of multilayered components, may contain residual solvents that pose a potential health risk due to their ability to migrate into food products. To address this concern, regulatory agencies have established strict limits on solvent migration and intake—limits that are largely modeled after those used in the pharmaceutical industry to ensure consumer safety.

This study presents the development and optimization of a headspace gas chromatography–mass spectrometry (HS-GC-MS) method for the detection and quantification of twelve residual solvents commonly found in packaging materials. Method parameters were fine-tuned using two columns (HP-5 and DB-1701), with DB-1701 demonstrating superior peak separation and resolution. Calibration curves showed excellent linearity ($R^2 > 0.9989$) across a concentration range of 1–250 ppm. Recovery rates ranged from 90% to 101%, and repeatability was confirmed with relative standard deviations around 5% for standards at 5 and 10 ppm. The method was successfully applied to real packaging samples from various food products, revealing the presence of ethanol, acetone, and isopropanol in several cases. This method enables efficient and reliable analysis of residual solvents in packaging materials, supporting compliance with international safety standards.

Keywords: residual solvents, food packaging, HS-GC-MS, regulative compliance.



Relationship Between Pigment Composition and Oxidative Stability in Camelina (*Camelina sativa* L.) Oil

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Camelina (*Camelina sativa* L) is a drought-tolerant oilseed crop valued for its short vegetative period and adaptability to low-quality soil. Its seeds contain 30–50% oil, rich in high polyunsaturated fatty acids (40–60%), and bioactive compounds such as phytosterols, tocopherols, carotenoids, chlorophylls, and phenolic compounds. Although these components contribute to the nutritional and functional quality of the oil, they can also affect its oxidative stability. This study aimed to evaluate the oxidative stability of oil obtained from two camelina genotypes (NS Slatka and NS Zlatka) grown at two locations in Serbia (Pančevo and Rimski šančevi) and to examine its correlation with β -carotene and chlorophyll content. The oxidative stability of the oil was evaluated using the Schaal Oven test. The peroxide value was determined at the beginning of test and after 4 and 8 days of incubation, while the β -caroten and chlorophyll contents were measured initially and after 4 days. All oil samples showed a progressive increase in peroxide value, ranging from 25.84 to 29.20 meq O₂/kg after 4 days and from 51.71 to 69.06 meq O₂/kg after 8 days, indicating intensive oxidation. Both genotype and growing location significantly influenced oxidative stability ($p < 0.05$). Higher peroxide values were recorded in genotype NS Zlatka (37.10 and 69.06 meq O₂/kg) compared to NS Slatka (29.20 and 54.36 meq O₂/kg) as well as in oils from both genotypes grown at the Rimski šančevi site. A decrease in pigment content accompanied the increase in peroxide value. Oils with higher initial β -caroten and chlorophyll levels generally exhibited greater stability, although this relationship was not consistent in all samples. The results highlight the influence of genotype and environmental conditions on the oxidative stability of camelina oil and underline the importance of natural pigments in maintaining oil quality during storage. These findings provide valuable insights for breeding programs aimed at developing camelina varieties with improved oil stability and quality.

Keywords: *Camelina sativa*, oil, oxidative stability, β -carotene, chlorophyll, peroxide value, genotype, growing location

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Optimization of Analytical Procedures for the Determination of OCPs and PCBs in Breast Milk

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Organochlorine pesticides (OCPs) and polychlorinated biphenyls (PCBs) are persistent organic pollutants (POPs) that resist environmental degradation. Due to their semi-volatility and lipophilicity, they are easily transported through air, water, soil, and food, and tend to bioaccumulate in living organisms. Long-term exposure to these compounds can cause various acute and chronic health effects, emphasizing the importance of monitoring their presence in biological matrices such as blood, urine, and milk.

Milk is a complex biological matrix rich in lipids, proteins, and carbohydrates, providing a suitable medium for the accumulation of lipophilic contaminants and serving as a valuable indicator of human exposure to these pollutants.

The aim of this study was to optimize a procedure for the extraction and analysis of 24 pesticides, including OCPs and PCBs, in human milk using gas chromatography coupled with an electron-capture detector (GC-ECD). Cow's milk was used for method optimization due to its availability and compositional similarity to human milk.

The optimization followed a "step-by-step" approach, including the evaluation of extraction mixtures (acetone/hexane at different ratios), protein denaturation agents (acetic acid and sodium acetate), purification steps (Florisil, alumina, and QuEChERS), and lipid removal using sulfuric acid added at different extraction stages. The acceptance criterion for method performance was recovery between 80% and 120%.

The optimized method, based on liquid-liquid extraction with hexane/acetone (50:50 v/v), cleanup with concentrated sulfuric acid and alumina column, and concentration using a Kuderna-Danish apparatus, ensures reliable recovery and quantification of target analytes and can support future national monitoring of human exposure to OCPs and PCBs through breast milk analysis.

Keywords: OCPs, PCBs, optimization, human milk, GC-ECD, step-by-step.



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SP – 6

Feasibility of Using Purple Phototrophic Bacteria for Valorization of Food Processing Waste

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Purple phototrophic bacteria (PPB) are photosynthetic microorganisms that use light energy and organic substrates as carbon and electron sources. Found in lagoons, sediments, and organic-rich wastewaters, they grow under anaerobic but illuminated conditions. Their metabolic versatility enables the conversion of various waste (lactose, volatile fatty acids, and carbohydrates) into valuable bioproducts like single-cell protein, biohydrogen, carotenoids, and polyhydroxyalkanoates, making PPB key agents for waste valorization and resource recovery in the circular bioeconomy. Their metabolic versatility makes them promising agents for waste valorization and resource recovery in the circular bioeconomy. Valorizing PPB biomass from wastewater into microbial protein provides a sustainable approach to resource recovery while enhancing food security in regions with limited agricultural productivity.¹ Advances in PPB metabolic engineering have expanded their applications in producing SCP and biohydrogen.² Moreover, PPB cultivation on dairy whey improves process economics by reducing substrate costs and generating high-value protein.³ Preliminary experiments show that PPB grown on diluted food industry wastewater achieved 60% protein content (w/w) and over 90% organic carbon removal after 72 hours of photofermentation. Overall, the reviewed studies demonstrate that PPB can transform organic waste streams into high-value bioproducts while reducing treatment costs and environmental impact. Continued optimization of large-scale bioreactor systems and market integration of PPB-derived products is essential to establish their commercial feasibility in food processing waste valorization.

Keywords: purple phototrophic bacteria, waste valorization, circular bioeconomy

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Development, Optimization and Testing of Silicone-Based Chemometers for Sampling and Quantification of Hydrophobic Organic Compounds in Water

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Rapid urban, industrial, and agricultural development in recent decades has increased water pollution, releasing a wide variety of contaminants into aquatic systems, with hydrophobic organic compounds (HOCs) being of particular concern. Their lipophilic nature may lead to bioaccumulation and biomagnification and can cause immune, reproductive, and endocrine disruption, posing risks to ecosystems and human health.

Assessing the bioavailable fraction of these pollutants is crucial for understanding their environmental fate and health implications. Conventional grab water sampling rarely reflects these fractions. Passive equilibrium sampling with silicone polymers offers an alternative to directly capture the bioavailable fraction, mimicking the chemical uptake in biota. However, reaching thermodynamic equilibrium with the sampler can take months to years for some compounds, due to slow mass transfer and resistance at the water–polymer interface. This research aimed to overcome these challenges and take a step forward in equilibrium sampling of HOCs in water using silicone chemometers, by optimizing sampler design. Glass jars, coated with silicone polymer layers of three different thicknesses, were deployed under pump-generated turbulent flow to accelerate the uptake by reducing the water boundary layer thickness. The newly developed silicone-coated jar samplers reached rapid equilibrium within 10 days for compounds with $\log K_{ow}$ values up to 6, demonstrating their potential for short-term field deployment and broad applicability across HOCs classes including polycyclic aromatic hydrocarbons, pesticides and personal care products.

Keywords: Silicone-based Chemometer, Passive Sampling, Hydrophobic Organic Compounds, Water Analysis



Green and Efficient Extraction of Phenolic Compounds from *Hypericum perforatum* using Natural Deep Eutectic Solvents

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Hypericum perforatum L. is a medicinal herb rich in various bioactive compounds, including procyanidins, phenolic acids, anthocyanins, xanthones, flavonoids, and naphthodianthrones. This study aimed to evaluate the selectivity of eco-friendly natural deep eutectic solvents (NADES) for extracting polyphenolic compounds from *H. perforatum* herbs and shoots.

Twenty NADES were prepared using choline chloride and betaine as hydrogen bond acceptors, combined with different donors such as organic acids (acetic, lactic, tartaric), carbohydrates (fructose, glucose, maltose, sucrose), urea, thiourea, glycerol, and sorbitol. Their extraction efficiency was compared with 70% methanol, a conventional solvent.

Phenolic compounds were identified and quantified using HPLC-DAD-MSⁿ. In herbs, flavonols were most abundant, followed by phenolic acids and xanthones, while in shoots, phenolic acids predominated. Organic acid-based NADES with choline chloride showed the highest extraction efficiency, followed by urea-based systems, whereas alcohol- and carbohydrate-based NADES were less effective. The choline chloride–lactic acid (1:1) mixture exhibited superior performance, yielding 76.35 mg/g and 120.4 mg/g for herb and shoot samples, respectively, comparable to 70% methanol (84.09 mg/g and 91.79 mg/g). The choline chloride–acetic acid (1:2) mixture also demonstrated high efficiency, with 74.77 mg/g in herbs and 95.47 mg/g in shoots.

These results highlight the potential of natural deep eutectic solvents as sustainable and efficient alternatives for extracting bioactive compounds from *H. perforatum*, supporting their further application in pharmaceutical research.

Keywords: NADES, *H. perforatum*, phenolic compounds, choline chloride, lactic acid.

Acknowledgement: This work has been supported by Macedonian Ecological Society for the financial support of the project titled “An ecological approach for the extraction of bioactive compounds from *Hypericum perforatum* using deep eutectic solvents”.



Comparative Study on the Efficiency of Natural Deep Eutectic Solvents for Phenolic Acid Extraction

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Natural deep eutectic solvents (NADES) are emerging as eco-friendly alternatives to conventional solvents, offering higher extraction efficiency and lower environmental impact. This study investigated the potential of nineteen NADES, synthesized from choline chloride in combination with organic acids, carbohydrates, urea, and glycerol, for the extraction of phenolic acids.

The solvents were characterized by FT-IR spectroscopy and evaluated for key physicochemical properties. They exhibited higher densities (1.13–1.40 g/mL) and surface tensions (35–88 mN/m) than water. Conductivity (36.1–8460 μ S/cm), adjustable pH (1–9), and elevated refractive indices (1.42–1.54) indicated high polarity, tunability, and strong solute–solvent interactions favorable for phenolic acid extraction.

Twenty phenolic acids, including coumaric, caffeic, ferulic, and their derivatives, were successfully extracted. Organic acid–based NADES demonstrated the highest extraction efficiency, followed by carbohydrate-based systems, whereas urea- and glycerol-based NADES were less effective. Among them, choline chloride–organic acid systems, particularly choline chloride–oxalic acid (1:1) and choline chloride–tartaric acid (2:1), achieved the best performance.

These findings highlight the importance of careful hydrogen bond donor/acceptor selection for tailoring NADES properties and optimizing phenolic acid extraction. Future studies should focus on fine-tuning NADES composition to target specific analytes and further improve extraction efficiency.

Keywords: NADES, extraction effectiveness, phenolic acids, pH

Acknowledgement: This work has been supported by Macedonian Ecological Society for the financial support of the project titled “An ecological approach for the extraction of bioactive compounds from *Hypericum perforatum* using deep eutectic solvents”.



Studies on Optimization Electrocatalytic Activity of Nickel Phosphides Towards Oxygen Evolution Reaction

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Nowadays, a huge global problem is climate change leading to increasing atmosphere pollution through the emission of carbon dioxide (CO₂)¹. The running out of non-renewable energy sources is driving scientists to look for better solutions to slow down the climate collapse.

The process of electrochemical splitting of water in two successive reactions: the oxygen evolution reaction (OER) and the hydrogen evolution reaction (HER), generates H₂ used directly as green energy. The selection of a suitable catalyst for these reactions is crucial, due to the limiting oxygen evolution reaction. Transition metal compounds are proving to be a decent, more affordable substitute of standard noble metal catalysts². They exhibit high catalytic activity, conductivity, good stability.

Therefore, the aim of this study was to synthesize a nickel phosphide based on a carbonized cellulose fiber, used as an electrocatalyst in the OER reaction, and to modify the obtained material with iron. The morphology of materials was investigated by various techniques. Electrochemical tests of the samples showed enhanced performance compared to the reference RuO₂.

Keywords: nickel phosphide, electrocatalysts, oxygen evolution reaction.

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SP – 11

Atmospheric Deposition of Chemical Elements and Microplastics in Mosses Around Industrial Zone of Kastriot in the Republic of Kosovo

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The aim of this study was investigation of chemical elements and microplastics in air of the industrial zone of Kastriot (Obiliq) in Kosovo, by using mosses as a bioindicator. Moss samples were collected during June 2025, from 6 locations in Kastriot and Fushë Kosova municipalities. Moss samples were digestion in Teflon tubes by using HNO_3 and H_2O_2 , and then 18 chemical elements (Al, As, Ba, Be, Cd, Co, Cr, Cu, Fe, K, Mg, Mn, Mo, Na, Ni, Pb, Se and Zn) analysed by Inductively Coupled Plasma Atomic Emission Spectroscopy (ICPE-9800). For determination of microplastics in mosses samples, 1 gram per each sample were digested by using Fenton reagent (ferrous iron sulphate solution 0.05 M) in the catalytic wet peroxide oxidation method¹. Samples were vacuum-filtered onto cellulose filter papers and placed into glass petri dishes for storage, and then analyzed for presence of microplastics using stereo-microscope². The basic statistics (minimum, maximum, mean, median, standard deviation and coefficient of variation), Pearson correlation, Cluster analyses, and Pollution indices (CF and PLI), used as a tool for analysing of data. The mean value of Contamination Factor (CF) revealed extremely high levels of pollution for Pb (333.1), Ni (20), Cr (18.1), Co (17.9), Fe (2.3), Cu (2.3), and Cd (1.99). The pollution load index (PLIsite) ranged from 8.73 to 13.22, and the PLI of a whole zone investigated was 10.88. In some mosses samples we identified the fibers and fragments of microplastics with dimensions from 800-2000 μm . These data of chemical elements and microplastics, indicating a significant of anthropogenic impact, because in this area are located the ferronickel open mines in Golesh, lignite mines and lignite power plants Kosova A and Kosova B in Kastriot, and also the heavy traffic in Pristina has a huge impact on air pollution with toxic metals³.

Keywords: Kosovo; air pollution; mosses; heavy metals, microplastics.

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Identifying and Eliminating Misconceptions Among Eighth Grade Chemistry Students

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This research investigates misconceptions in the teaching of chemistry to eighth-grade students by analyzing results from a municipal chemistry competition. The competition was designed to promote critical thinking and focused on core chemistry topics, including states of matter, metals and nonmetals, simple substances, compounds, and mixtures. The research sample included 506 eighth-grade students. Data within this research were obtained through the analysis of tests implemented during the competition and the corresponding Excel tables with student results. The analysis was conducted using Gilbert's criterion,¹ which categorizes students' conceptual understanding into four levels: good, satisfactory, insufficient, and completely unacceptable. Particular attention was given to incorrect answers (distractors) chosen by more than 20 % of students, as these are indicative of the presence of misconceptions.² Misconceptions in chemistry can significantly hinder students' comprehension of fundamental concepts. Based on the students' responses, a total of 13 misconceptions were identified. These findings underscore the importance of continuous, targeted instruction to effectively address and correct misunderstandings in chemistry.³

Keywords: chemistry competition; curriculum; conceptual understanding; misconceptions.

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Optimization of a Lab-Scale Synthetic Method for Quinacridone Derivatives and Their Characterization

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Quinacridones are a class of fluorescent compounds sharing an aromatic structural motif, and as such, they can be employed as fluorophores when using both visual and instrumental techniques, especially for the research of biomolecules (DNA, RNA, saccharides, etc.). These compounds have a special advantage over other fluorophores, as they provide a solution to the problem posed by the autofluorescence of biomolecules in the blue area of the electromagnetic spectrum. This can cause interference if techniques relying on blue-emitting fluorophores are used. Namely, this problem can generally be solved using higher wavelength emitting fluorophores, a criterion for which these compounds are a good match.

This study offers a relatively fast and simple synthetic method, involving derivatization of the starting material (basic structural motif of the desired compound) by simplifying the variation of the derivatives' substituents. Diethyl succinate is used as a starting material, while the specific derivatives are obtained by reacting diethyl succinyl succinate with an appropriate arylamine. The synthetic steps were optimized, and the reaction was monitored by TLC. The derivatives are characterized using UV-VIS spectroscopy, powder XRD, vibrational spectroscopy (IR and Raman), and NMR. The fluorescence of the compounds is observed under UV light.

Twenty-three novel fluorescent compounds were synthesized, and several trends were observed. A correlation between optoelectronic properties and the electron donating or withdrawing effect of the substituents was identified and analysed. The effect of hydrogen bonding and extended aromatic systems was also studied.

Keywords: quinacridone, PXRD, fluorescence, vibrational spectroscopy, NMR



Design and Implementation of a Python Tool for Multi-Method Calibration in the Quantitative Analysis of Organochlorine Contaminants using Gas Chromatography

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Organochlorine pesticides (OCPs), chlorobenzenes (CBs) and polychlorinated biphenyls (PCBs) are persistent organic pollutants characterized by high environmental stability and bioaccumulation. Although their use has been restricted, residues are still frequently detected in water, sediments, and biota as a result of intensive agricultural practices in the past and inadequate waste management.

This work represents an important segment in the implementation of a method for monitoring OCPs, CBs and PCBs in the Vardar River using GC-ECD. There are several approaches used for calibration in quantitative analysis of multiple target compounds that have been optimized here by creation of a calibration application to reduce analysis time and potential human errors in manual data processing. It supports three calibration approaches: single-point calibration with an internal standard, multi-point internal calibration curve, and external calibration curve. The tool was developed in Python, using the Streamlit framework for an interactive interface. It offers a faster, more transparent, and reproducible workflow, also suitable for future environmental analyses of similar contaminants. It was successfully applied in the study of 36 organochlorine contaminants in water samples by direct extraction of retention and peak height data for the 36 target compounds from the chromatograms of the standards and sample extracts most efficiently and accurately.

Keywords: organochlorine contaminants, quantitative analysis, calibration, Python

Acknowledgment: The financial support received through a student grant from the University Student Assembly of UKIM is gratefully acknowledged.



Introduction and Application of an Analytical Method for Monitoring Organochlorine Contaminants in the Vardar River Using Gas Chromatography

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Organochlorine pesticides, chlorobenzenes and polychlorinated biphenyls represent groups of persistent organic pollutants (POPs) highly resistant to degradation. Due to their chemical stability and lipophilic nature, they tend to accumulate both in the environment and in biological systems. Given their historical use in agriculture and industry, the Vardar River was selected for assessing potential residual contamination. Surface water samples were collected from eight representative sites to evaluate their presence and distribution along the river path. Liquid–liquid extraction with petroleum ether was used for sample preparation, and analyses were carried out using GC-ECD for quantification and GC-MS for identification.

The analysis revealed that hexachlorocyclohexane (HCH) isomers were still detectable across multiple locations. Polychlorinated biphenyls were mostly abundant in the midstream region (Bashino Selo and Nogaevci), while the downstream sites showed lower values. In addition to target analytes, qualitative screening indicated the presence of long-chain hydrocarbons, alcohols, and phthalates, pointing to a mixture of natural organic matter and diffuse anthropogenic inputs.

These findings confirm the ongoing persistence of organochlorine pollutants within the Vardar River basin and underline the necessity of continuous environmental monitoring.

Keywords: organochlorine contaminants, GC-ECD, GC-MS, Vardar River, POPs

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Antimicrobial Properties of Silver Nanoparticles Impregnated in Socks Using Fruit Waste Grape

Pomace

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Each year, the global wine industry generates approximately 12 million tons of grape waste (pomace), which poses a significant environmental threat due to the presence of residual chemicals from grape cultivation and winemaking. These chemicals can leach into soil and water, increasing soil acidity and contaminating groundwater. Our project aims to address this issue by repurposing grape waste into a valuable material for the medical field.

In response to the growing problem of chronic wound infections and antibiotic-resistant bacteria, we developed a novel method to create antibacterial socks by combining grape waste materials with silver nanoparticles (AgNPs). Silver nanoparticles are known for their strong antibacterial properties, and our approach offers an environmentally friendly and cost-effective method of integrating them into textiles.

The antibacterial effectiveness of the socks was tested at the Institute of Microbiology and Parasitology, Faculty of Medicine, Ss. Cyril and Methodius University in Skopje. The socks were evaluated against *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Escherichia coli*, *Bacillus subtilis*, and *Candida albicans*, showing significant inhibition of bacterial growth.

This innovation holds particular promise for medical applications, such as wound care for diabetic patients, where infection prevention is essential for healing. Additionally, our method reduces production costs and environmental impact compared to conventional techniques like UV treatment, making it a sustainable and affordable solution.

This project demonstrates how agricultural waste can be transformed into high-value medical products, contributing to both environmental sustainability and public health.

Keywords: silver nanoparticles, grape pomace, impregnated socks, antibacterial properties, wound healing, reducing waste

Uncomplex Outcomes: Spontaneous Oxidation of 2-(diphenylphosphino)benzaldehyde Schiff Base

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Our recent research focuses on the reactions of the Schiff base 2-(diphenylphosphino)benzaldehyde with 3-nitrophenylhydrazine, yielding the condensation product **L**, and its coordination behaviour with different transition metals. In an initial try **L** reacted with CuBr₂ (1:1 molar ratio) in a warm MeOH solution of CuBr₂ and a warm CH₂Cl₂ solution of **L**. Upon cooling to room temperature dark orange crystals were obtained. Their analysis (FT-IR and single-crystal X-ray diffraction) confirmed a oxidation of **L** to **Lox** had occurred (Figure 1). The purity of the product was verified by elemental analysis (C, H, N). Although coordination was not achieved, the obtained results allow for a comparative structural analysis of the unoxidized and oxidized ligand form, contributing to a better understanding of structure–property relationships. These insights will support the design of further ligands and their metal complexes with tailored characteristics.

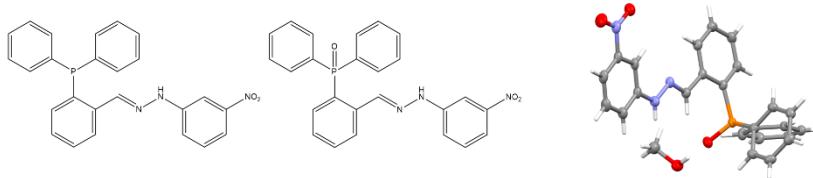


Figure 1 Structural formula of **L** (a), **Lox** (b) and ORTEP of molecular structure **Lox·MeOH** (c)

Crystallographic data: monoclinic crystal system, $C2/c$, $a = 30.7578(6)$, $b = 9.2135(2)$, $c = 21.2589(4)$ Å, $\beta = 129.030(1)$, $V = 4679.92(17)$ Å³, $Z = 8$. Refinement based on F^2 (316 parameters): $R_1 = 0.0423$, $wR_2 = 0.1004$, $S = 1.095$, for all data, and $R_1 = 0.0370$ for 4776 reflections with $I \geq 2\sigma(I)$.

Keywords: synthesis, single crystal X-ray study, FT-IR, elemental analysis, oxidation



ZnO/GO-Modified Glassy Carbon Electrode for Electrochemical Sensing of Doxorubicin

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Doxorubicin (DOX), a widely used anthracycline chemotherapeutic drug, poses environmental risks due to its persistence and toxicity, creating a need for rapid and sensitive detection techniques. In this context, electrochemical sensors (ECS) have emerged as efficient tools for DOX detection, offering high sensitivity, selectivity, and fast response. The performance of such sensors can be further enhanced by modifying the electrode surface to facilitate charge transfer and improve detection efficiency.

In this work, ZnO/GO composites with 0.01 and 0.05 wt% GO were synthesized via microwave processing of Zn(OH)₂ precipitate and used as electrode modifiers for DOX detection. The physicochemical properties of the ZnO/GO composites were characterized using X-ray powder diffraction (XRD), Raman and Fourier-transform infrared (FTIR) spectroscopy, field emission scanning electron microscopy (FESEM), UV–Vis diffuse reflectance spectroscopy (DRS), and photoluminescence (PL) spectroscopy. Cyclic voltammetry (CV) was used to study the electrochemical response of DOX on a ZnO/GO-modified glassy carbon electrode. CV measurements were carried out in 25 mL of phosphate buffer solution (0.1 M, pH 7.0) with successive additions of doxorubicin infusion solution (Ebewe Pharma, 50 mg DOX / 25 mL) in portions ranging from 10 to 350 µL. All experiments were performed within the potential range of –0.4 to 0.6 V at a scan rate of 50 mV·s^{–1}. Electrochemical sensitivity of ZnO/GO composites toward DOX was correlated with their physicochemical characteristics.

Keywords: electrochemical sensors, zinc oxide, graphene oxide, doxorubicin

Acknowledgement: The authors KA, AS, ISS, and SM acknowledge the financial support from the Science Fund of the Republic of Serbia, The Program PRISMA, #7377, Water pollutants detection by ZnO-modified electrochemical sensors: From computational modeling via electrochemical testing to real system application – WaPoDe.



Siloxane Film Investigation on Modified Silicate Glass Obtained from TEOS In Water/Toluene Solution

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Soda-lime-silica glass is commonly used in both industrial and household settings due to its transparency, chemical resistance, availability and environmental friendliness. Enhancing the glass surface hydrophobic properties is sometimes necessary, as in the case of self-cleaning surfaces. This study investigates the surface modification of soda-lime-silica glass using tetraethyl orthosilicate (TEOS), dissolved in wet toluene (water/toluene) and employing dip-coating method.

Several techniques and methods were used in the investigation of the modified glass surface: specular reflectance FTIR spectroscopy, contact angle measurements, obtainment of the isoelectric point using streaming potential, and AFM microscopy.

Our findings demonstrate successful functionalization of soda-lime-silica glass surface and formation of siloxane film using TEOS as precursor. The obtained film possess specific morphology, producing high water contact angle close to 90 ° and thus close to being hydrophobic. This result shows how the surface film design and properties might depend not only on the silane, but also on the solvent used.

Keywords: TEOS, hydrophobic, FTIR, contact angle, AFM, glass



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SP – 20

Tribocatalytic Degradation of Cephalexin by Sol-Gel ZnO Powders: Effect of the Solvent

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Cephalexin is an organic compound and an antibiotic that often pollutes the environment and needs to be removed. It is commonly found in hospital waste, agricultural runoff, and drinking water. Because it does not decompose easily, removal is necessary. The most effective and environmentally friendly method for removing Cephalexin is tribocatalysis, which is a self-powered process that requires neither light nor heat. It relies solely on mechanical energy generated by rubbing the catalyst on the surface of the Cephalexin. The degradation rate of Cephalexin varies depending on the solvent used. From tribocatalytic tests, it is evident that using methanol as a solvent in the sol-gel synthesis of ZnO for Cephalexin degradation is more efficient, achieving 73% degradation, compared to ethanol, which reaches a maximum efficiency of 58%. Both tests used a polytetrafluoroethylene (PTFE) beaker. Additionally, increasing the rotations of the magnetic stirrer can improve degradation; more rotations create friction between the PTFE beaker and the catalyst, leading to increased electron absorption by the beaker and the formation of more positive holes on the catalyst, which enhances the oxidation of Cephalexin. Tribocatalysis is a relatively new and promising method for oxidatively removing pollutants. It provides an environmentally friendly solution by converting mechanical energy into chemical energy for pollutant degradation.

Keywords: Tribocatalysis, ZnO, Cephalexin, degradation

Acknowledgment: Nina Kaneva is grateful to be financially supported by the Bulgarian NSF project KP-06-N89/07 (КП-06-Н89/07).



Perspectives on the Utilization of Waelz Clinker

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Waelz clinkers (slags), generated during the thermal treatment of zinc-bearing secondary resources in rotary kilns, represent a significant stream of industrial waste containing iron, calcium, silicon, and other valuable components. However, on a global scale, a large proportion of these materials are still landfilled, posing both environmental and economic challenges^{1,2}. The limited capacity for landfilling, the high cost of disposal, and the strict requirements for the handling of hazardous waste necessitate the development of sustainable solutions based on the principles of the circular economy.

Based on theoretical analysis, literature data, and preliminary laboratory results, this paper outlines recycling and metallurgical valorization routes for Waelz clinkers. Approaches include pyrometallurgical recovery of iron and other metals³, as well as use in construction materials and ceramic products. Laboratory studies showed variations in composition, phases, and porosity, determining their suitability for specific applications: iron-rich slags with high magnetic fractions are suitable for metallurgical reuse, while silicate- and calcium-rich types fit construction and composites. These results highlight Waelz clinker as a resource with multiple utilization pathways.

Further thermodynamic and thermogravimetric studies are essential for developing efficient and sustainable technologies.

Keywords: Waelz clinker, utilization, secondary raw materials, recycling, metallurgy

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Investigation of Siloxane Film on Modified Silicate Glass Obtained from TEOS In Dry Toluene Solution

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Soda-lime-silica glass is widely utilized in industrial and domestic applications. In certain cases, changes in the surface properties are needed. This study investigates the surface modification of soda-lime-silica glass using tetraethyl orthosilicate (TEOS) dissolved in dry toluene and employing dip-coating method.

The modified surfaces were characterized using a range of analytical techniques and methods: contact angle measurements, ratio-reflectance and two trace two dimensional (2T2D) correlation spectra obtained from the measured specular-reflectance Fourier Transform Infrared (FTIR) spectra and isoelectric point, to evaluate alterations in surface charge. Additionally, atomic force microscopy (AFM) was used to examine the surface morphology.

Results indicate successful glass surface modification with TEOS and interesting morphology of the film, leading to a very small increase in the water contact angle of about 10° from that of the pure glass. These findings suggest that glass surface modification with TEOS from dry toluene as solvent, covers and shields the glass surface, while retaining the hydrophilicity.

Keywords: TEOS, Dry-toluene, Specular Reflectance, Contact angle, siloxane film



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SP – 23

Revisiting the Nucleation of High-Entropy (Oxy)(hydr)oxides

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High-entropy (oxy)(hydr)oxides have been recently proposed as promising materials for environmental remediation and electrocatalytic applications due to their ability to integrate multiple cations into a single structure. This compositional complexity generates synergistic effects that outperform those of single-metal systems. However, current synthesis methods largely overlook the chemical and hydrolysis behavior of particular metals, introducing uncertainties to the final functional performance of these materials. This study focuses on the existing synthesis strategies, emphasizing the chemistry of single metals (Fe, Ni, Co) constituting typical high-entropy (oxy)(hydr)oxides. Special attention is given to the heterogeneous nucleation and the influence of substrate properties, including chemical composition, crystal structure, and functional groups, on the nucleation, growth, and particle morphology, providing fundamental insights into the nucleation behavior and paving the way toward the rational design of high-entropy (oxy)(hydr)oxides as efficient and sustainable solutions for modern societies.

Keywords: nucleation; homogeneous; heterogeneous; hydrolysis, high-entropy (oxy)(hydr)oxides; iron; nickel; cobalt; electrocatalysis; environmental remediation;



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SP – 24

Draping Different Styles of Women's Clothing

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The aim of the paper is investigation of the draping behavior of different styles of women's skirts. The relationship between the garment draped area from various sides, mounted on a dummy, and the physical-mechanical properties of the textiles (drape coefficient, thickness, and GMS) was investigated. Two styles of women's skirts were constructed from fabrics having various fabric weights (157.6 to 296.5 g/m²). The styles constructed were a full circle skirt style and had identical cut lengths. The styles were mounted on a mannequin, and their appearance and draping were photographed from all sides. The drape coefficient (DC) of the fabrics used for garment construction ranged between 46.5 and 93.6%. The investigations show positive correlations between the DC and the GSM of the materials (0.76) and between the fabric thickness and the GSM (0.71). The draped areas of the garments from four sides were analysed from the photographs using image analysis. The garment styles investigated show differences regarding the draping profile and correlation between draping areas and fabric physical properties, as well as between the number of nodes (N_n) and the various side draped areas. The correlation between the draped areas of the front side and the areas of the other three sides, for the full circle style is high (0.96 - 0.98), while the 1/2 circle style shows correlation values from 0 to 0.7.

Keywords: drape, GSM, skirt, correlation, garment appearance

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Optimization Of Cop Diameter in Ring Spinning Process Using Statistical Taguchi Method

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The ring-spinning process is an important manufacturing process for the mass customization of clothing goods, especially for large-run yarns. Cop quality is one of the most important characteristics concerning ring-spun yarns. It is mainly evaluated and compared via the diameter of a cop. This study aimed to optimize the ring spinning parameters influencing the cop diameter. The optimization of the spinning process was investigated using the statistical Taguchi method. The diameter of the cop in the ring-spinning process was characterized and evaluated based on the variation in traveler mass (factor K with levels: 60, 67.5, and 75 mg), spindle speed (factor L with levels: 12900, 13300, and 13700 min⁻¹), and doff stage (factor M with levels: 43, 111, and 179 mm). It was concluded that changing the doff stage over the cop had a severe effect on the diameter of the cop which gave a recommendation for engineering design too but the cop optimum diameter for the manufacturers and researchers. Traveler mass and spinning spindle had no effect. The optimization method of Taguchi gave a reasonable result to the maximum cop diameter corresponding to the specimen and test condition. According to the proposed levels of the control factors, it was concluded that the maximum cop diameter at the bottom ring rail position could be achieved at factor level K1L1M2, with a traveler mass of 60 mg, spindle speed of 12900 min⁻¹, and doff stage of 111 mm. Using the S/N ratio, the best combination of factor levels that yield the highest value of cop diameter was detected efficiently.

Keywords: Taguchi method, yarn, cotton, optimization

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Nitrogen-Modified Pyrene Scaffolds as a Platform for New Luminescent Materials

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The design of advanced luminescent materials increasingly relies on heteroatom-containing aromatic systems with finely tunable optical properties. Among these, pyrene derivatives and their isosteres, particularly azapyrenes, offer promising structural motifs for applications in organic electronics. This study presents the development of a synthetic strategy and the comprehensive characterisation of 2,7-diazapyrene and related derivatives. Target compounds were obtained, including unsubstituted 2,7-diazapyrene, non-K substituted pyrenes and non-K and K-region substituted diazapyrenes. Efficient synthetic routes were established using microwave-assisted procedures affording the desired products in satisfactory yields. The compounds were characterized by ¹H and ¹³C NMR and FTIR spectroscopy, while their thermal behavior was investigated using TGA and DSC. Particular emphasis was placed on photophysical studies, including UV–Vis absorption and emission spectroscopy under varying solvent polarity. Experimental observations were supported by DFT and TD-DFT calculations, providing insights into molecular geometries, frontier orbital distributions, and electronic transitions. The results reveal that nitrogen incorporation into the pyrene scaffold significantly alters electronic structure and emissive properties, while substitution patterns in the non-K versus K regions modulate band gaps, dipole moments, and molecular planarity. These findings highlight diazapyrenes as a versatile platform for the development of next-generation luminescent materials.

This research was funded by the National Science Centre, Poland, under the SONATA programme, grant no. 2023/51/D/ST5/00369.

Keywords: Pyrene, Azapyrene, Donor–acceptor systems, Photophysical properties, Fluorescence



Synthesis and Characterization of Aminoguanidinium Lead, Bismuth, and Antimony Iodide Perovskites

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The organic-inorganic perovskites (HOIPs) have attracted significant attention as promising new materials for their broad applications, particularly in photovoltaics. Their use as materials for the construction of solar cells is particularly sought-after, given their relatively simple synthesis, low production cost, and environmental compatibility. In this study, the synthesis and characterization of bulk samples and thin films of new hybrid iodide perovskites with aminoguanidinium (AGu^+) as the organic cation, paired with different inorganic cations (Pb^{2+} , Bi^{3+} , and Sb^{3+}), is presented.

Aminoguanidinium lead iodide was synthesized by dissolving lead iodide and a pre-synthesized aminoguanidinium iodide precursor in a minimal amount of dimethylformamide (DMF), followed by the Antisolvent Vapor-Assisted Crystallization method. Aminoguanidinium bismuth iodide and aminoguanidinium antimony iodide were synthesized by dissolving a mixture of aminoguanidinium bicarbonate and the respective inorganic compound (Bi_2O_3 or SbI_3) in concentrated hydroiodic acid. The solution was cooled down to induce crystallization. Thin films of the substances were prepared using the spin coating technique.

The obtained perovskites were characterized by PXRD at room temperature and infrared spectroscopy in a wide temperature range (from -170 °C to 250 °C). The thin films were analyzed with UV-VIS spectroscopy, from which the direct and indirect band gaps were determined.

Keywords: hybrid iodide perovskites, aminoguanidinium, PXRD, perovskite solar cells



Exohedrally Functionalized Singlewalled Carbon Nanotubes in Oxygen Evolution Reaction

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In this study, pristine single-walled carbon nanotubes (SWCNTs) and SWCNTs functionalized with NiO compounds via an exohedral route were investigated as electrocatalysts for the oxygen evolution reaction (OER). Microscopic analysis revealed bundles of pristine SWCNTs decorated with NiO nanoparticles. Linear sweep voltammetry showed that SWCNTs_NiO and SWCNTs_pristine exhibited lower overpotentials (325 and 373 mV, respectively) compared to commercial RuO₂ (376 mV). Chronopotentiometry was used to study the relationship between overpotential and current density over time, allowing determination of Tafel slopes. SWCNTs_NiO showed the lowest Tafel slope (117 mV/dec), indicating enhanced kinetics. Extended stability tests revealed excellent long-term performance: SWCNTs_pristine showed negligible potential increase at 10 and 20 mA/cm² and only 5.3% at 50 mA/cm², while SWCNTs_NiO also outperformed RuO₂. These results demonstrate that SWCNTs are efficient hosts for electroactive species, improving both conductivity and stability.

Keywords: Singlewalled carbon nanotubes, exohedral functionalization, electrochemical water splitting, oxygen evolution reaction (OER)

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3D Assemblies of NiO NPs: a Precursor-Modulated Nanoscale-Engineering Approach Based On Turbostratic Ni₃(OH)₄(NO₃)₂ and Ordered β-Ni(OH)₂ Intermediates

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A surfactant free ammonia and carbamide precursor-modulated nanoscale-engineering of self-assembled flower-like 3D NiO nanostructures, based on ordered β-Ni(OH)₂ and turbostratic Ni₃(OH)₄(NO₃)₂ nanoplate structured intermediates, is reported. Employing a variety of complementary structural and spectroscopic techniques, fundamental insight into the structural transformation from intermediates to NiO NPs is provided.

The two sets of NiO NPs have distinct morphology, size, optical, electrical and surface properties which were characterized using XRD, SAED, TEM, HRTEM, SEM, AFM, UV-VIS and DSC. β-Ni(OH)₂ NPs and Ni₃(OH)₄(NO₃)₂ NPs are nanoflake-like and are self-assembled in flower-like nanostructures. The structure of β-Ni(OH)₂ NPs is high-ordered, while Ni₃(OH)₄(NO₃)₂ NPs are turbostratic. According to DSC analysis, the phase transition from Ni₃(OH)₄(NO₃)₂ to NiO NPs goes through two steps at 306 °C and 326 °C corresponding to free interlayers ions and H₂O species loss, followed by loss of chemically bonded OH⁻ and NO₃⁻ ions. Transformation to NiO NPs via ammonia route proceeds as a single phase-transition, accompanied with loss of OH⁻ species at 298 °C.

Ammonia derived NPs keep the nanoflower morphology by self-assembly into nanoplates, enabled by H₂O mediated adhesion on the NiO NPs {100} neutral surfaces. Structural transformations of turbostratic Ni₃(OH)₄(NO₃)₂ nanoplates result in formation of NiO NPs dominantly shaped by inert polar OH terminated (111) atomic planes, leading to loss of initial self-assembled 3D structure. Carbamide derived NiO NPs are three times larger, have larger band gap energy, more concentration of nickel vacancies, larger p-type conductivity and polar surfaces compared with NiO NPs prepared using ammonia.

The choice of the precursor defines the properties of nanoparticles providing pathways of utilizing them as p-type material and allows precise nanoengineering of polar and neutral surfaces dominated NiO NPs which is of exceptional importance in catalysis.

Keywords: NiO NPs, flower-like morphology, nanoplates, nanorods, annealing-induced phase transformation.



Synthesis and Characterization of Morpholinium Lead, Bismuth and Antimony Iodide Perovskites

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Hybrid organic-inorganic perovskites (HOIPs) have become a widely studied class of compounds since the synthesis of the “revolutionary” compound $(\text{CH}_3\text{NH}_3)\text{PbI}_3$, which, as a result of its optoelectronic properties, paved the way for more extensive research towards the synthesis of this type of compounds. Due to their promising properties and potential applications in the construction of diodes, photosensors, and photovoltaic cells, interest in HOIPs has grown exponentially over the past two decades.

In this work, HOIPs with morpholinium as the organic cation and I^- as the anion were synthesized and characterized. In order to monitor the changes in the structure and the influence on the optoelectronic properties, different cations (Bi^{3+} , Sb^{3+} , and Pb^{2+}) were used during the synthesis. The composition of the synthesized compounds was determined by elemental CHN analysis and EDXS. The crystal structures were determined and investigated by powder and single-crystal X-ray diffraction. The characterization of the obtained compounds aimed at determining their applicability as semiconductors, based on the direct and indirect energy widths of the forbidden band.

Further, the compounds were investigated by Raman spectroscopy and infrared spectroscopy in the mid- and far-infrared regions from -170 to 250 $^\circ\text{C}$. The phase transformations of the compounds were determined by differential scanning calorimetry. Thin films of the substances were prepared using the spin coating technique and analyzed by UV-VIS spectroscopy, the obtained data were used to construct Tauc diagrams from which the energy bandgap widths were determined.

Keywords: hybrid organic-inorganic perovskites, morpholinium, PXRD, SCXRD, infrared spectroscopy, UV-VIS spectroscopy



Structural and Electrical Characterization of Graphene/PVC and Graphene/PMMA Composites for EMI Shielding in Smart Buildings

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The increasing number of wireless devices and sensitive electronics in modern smart buildings requires strong protection against electromagnetic interference (EMI). Traditional metallic shields are often too heavy and vulnerable to corrosive degradation. Polymer composites reinforced with conductive nanomaterials, such as graphene, offer a superior alternative due to their high electrical conductivity, mechanical flexibility, and low density. This study investigates the critical dependence of EMI shielding effectiveness (SE) on both the selection of the polymer matrix (polyvinyl chloride, PVC, and poly(methyl methacrylate), PMMA) and the specific graphene loading concentration (0.3 *wt. %* and 1.0 *wt. %*). The resulting composite films were thoroughly characterized using Raman spectroscopy, Thermogravimetric Analysis/Differential Scanning Calorimetry (TGA/DSC), X-Ray Diffraction (XRD), Transmission Electron Microscopy (TEM), and dielectric measurements. These structural and electrical analyses were performed to establish the precise relationship between the composite's microstructure (including graphene ratio and dispersion), its thermal stability, and the formation of a critical conductive network necessary for effective EMI shielding. Key findings indicate that PMMA/G nanocomposites exhibit a significantly higher mass residue (~75 %) compared to PVC/G (~10 %), which is crucial for maintaining a conductive network and structural integrity under high temperatures. The obtained data provide essential insights into the optimal design parameters for engineering effective, scalable polymer-graphene shields.

Keywords: Graphene, PVC, PMMA, Composite, Films, EMI Shielding



Preparation and Analysis of Two Layered Coating on Silicate Glass

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The surface of silicate glass can be modified with various organosilanes to obtain a hydrophobic surface, thereby enhancing water repellency without compromising transparency. The modification of glass surfaces involves the formation of a nanofilm using hydrophobic materials and increasing the surface roughness. Experiments were performed with hydrolyzed and non-hydrolyzed 3-aminopropyltriethoxysilane (APTES), with or without the addition of sodium dodecyl sulfate (SDS) as a second layer. One common feature for all experiments was the low concentration of APTES and SDS (0.01 M). Previous investigations using high concentrations of APTES produced a hydrophobic glass surface.¹ The modified samples were analyzed using infrared (IR) spectroscopy, two-trace two-dimensional correlation spectroscopy (2T2D-COS)² and atomic force microscopy (AFM). Contact angle and surface energy measurements were evaluated through employing a drop shape analyzer. The results demonstrated successful silanization of the surface, obtaining a contact angle of 70–80°.

Keywords: silicate glass, hydrophobicity, silane, APTES, IR specular reflectance, 2T2D-COS, contact angle, AFM

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Synthesis of Lignin/TiO₂ Waterborne Polymer Composites

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Waterborne polymers are widely used in many fields primarily due to their eco-friendliness, versatility and good film forming properties, but drawbacks related to their mechanical properties and stability are still present. To enhance the properties of the waterborne polymer system, lignin and lignin/TiO₂ hybrid fillers (1:1 w/w) were incorporated into a butyl methacrylate–methyl methacrylate matrix. The fillers were added in the composite in concentration of 5 wt%. Additionally, to investigate the effect of the lignin/TiO₂ concentration, a composite containing 10 wt% lignin/TiO₂ hybrid filler was prepared. Composite preparation was carried out via emulsion mixing, where the pre-synthesized polymer matrix served as the dispersion medium, and the filler was introduced dropwise under continuous agitation. The hybrid filler, as well as the composites were analyzed using UV-Visible spectroscopy. The results indicated that the incorporation of TiO₂ led to significant absorption of UV and visible light, which makes the lignin/TiO₂ filler efficient UV-shielding agent. To investigate the UV stability of the composites, they were subjected to accelerated UV aging (254 nm, 50 °C, 50% RH, 264 h). The progress of UV aging was followed through infrared spectroscopy. These results revealed that a higher concentration of the hybrid filler is most efficient at reducing photooxidative degradation of polymer composites. Thermogravimetric analysis showed that incorporation of lignin and lignin/TiO₂ filler shifted the maximum degradation temperature to a higher value, improving the thermal stability of the composites. These findings demonstrate that lignin/TiO₂ hybrid fillers can improve the overall durability of polymer composites.

Keywords: Waterborne polymers, lignin/TiO₂, UV-stability



Theoretical IRMPD Spectroscopy of Hydrogen- and Helium-Tagged Protonated Glycine

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This work presents an exact theoretical model aiming to provide in-depth insights into IRMPD spectroscopic data of free and tagged protonated glycine, the simplest amino acid and a benchmark system for understanding fundamental intramolecular interactions in biomolecules. Infrared multiple photon dissociation (IRMPD) spectroscopy, supported by advanced quantum-mechanical calculations, was used to explore its structural, vibrational, and dynamic behavior in the gas phase and in microsolvated or tagged complexes.

Calculations were carried out at the density functional theory (DFT) level using hybrid and dispersion-corrected functionals. Anharmonic frequency analyses based on computation of the vibrational potentials and sequential solution of the vibrational Schrödinger equation reproduced experimental IRMPD spectra with high fidelity and enabled reliable assignment of key O–H and N–H stretching and bending modes.

Temperature-dependent simulations, performed via Boltzmann-weighted averaging over 4–40 K, revealed that at cryogenic conditions protonated glycine occupies its lowest-energy conformers, while at higher temperatures it undergoes interconversion among nearly isoenergetic structures. Molecular tagging with He and H₂ stabilizes the ions and enhances spectral resolution, causing subtle frequency shifts associated with weak hydrogen-bond perturbations.

Overall, the integration of high-resolution spectroscopy and quantum-mechanical modeling provides a coherent interpretation of protonated glycine's structure and dynamics, offering a framework for future studies of proton transfer and microsolvation in biomolecular ions.

Keywords: Protonated glycine; IRMPD spectroscopy; Density Functional Theory; anharmonic vibrations; conformational isomerization; hydrogen bonding; molecular tagging; microsolvation.



Following the Phase Transition and Vibrational Dynamics in Ibuprofen by Temperature-Dependent Infrared Spectroscopy in Conjunction with 2D Correlation Analysis

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Two-dimensional correlation spectroscopy (2DCOS) is a powerful technique for investigating structural changes initiated by some external perturbation. In this study 2DCOS analysis was applied to temperature-dependent FTIR spectra of ibuprofen powder, over the spectral region 500-2000 cm⁻¹. This region covers key vibrational modes such as aromatic, carbonyl and C–O stretching vibrational modes. The main focus of this study is monitoring the structural dynamics across the melting region of the sample. Using moving window 2D correlation spectroscopy (MW2DCOS) the melting temperature interval was identified, along with the vibrational bands exhibiting the most significant changes during the melting process. Generalised 2D infrared correlation spectra were also generated providing enhanced resolution of overlapping vibrational bands and enabling chronological tracking of vibrational mode changes. The methodology offers a promising tool for characterizing melting and other phase transition behavior, as well as monitoring the structural dynamics in pharmaceutical crystals.

Keywords: 2DCOS, MW2DCOS, ibuprofen, FTIR, phase transitions, molecular dynamics.



Theory of THz Spectroscopy of Liquid Water

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A combined molecular dynamics – quantum mechanical model was developed, aiming at understanding of the THz spectroscopy of bulk liquid water. Classical molecular dynamics simulations, based on many-body interaction potentials derived specifically for water, were used to generate snapshots which were further subjected to quantum mechanical DFT calculations.

Selected clusters from 100 MD snapshots were chosen such as to include: i) all the water molecules from the first hydration shell around randomly chosen water molecules, embedded in bulk water treated as a polarizable continuum; ii) all the water molecules from the first and second hydration shells around randomly chosen water molecules, embedded in bulk water treated as a polarizable continuum; iii) series of clusters involving sequentially increasing number of water molecules around randomly chosen one, embedded in a polarizable continuum. Partial geometry optimizations for all mentioned clusters were performed, fixing different regions of the shell structure, followed by computation of the second derivative matrices and harmonic vibrational frequencies at HCTH/aug-cc-pVTZ level of theory.

Excellent agreement was obtained between the results generated from the developed theoretical model and the experimental THz spectroscopic data.

Keywords: water, THz spectroscopy, DFT, molecular dynamics.



Validation of Greenness UV Spectrophotometric Method for Determination of Ciprofloxacin in Citeral® Eye/Ear Drops

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A UV spectrophotometric method was validated to determine ciprofloxacin (CIP) in Citeral® eye/ear drops. A 0.1 mol/L HCl solution was used as a solvent for preparing standards and samples. The spectra of the samples were recorded in the range of 240–400 nm. The method demonstrated linearity in the range of 0.1–20 µg/mL, with a correlation coefficient exceeding 0.99999, obtained from absorption measurements at three wavelengths (277, 316, and 330 nm). The LOD and LOQ values at 277 nm were 0.10 µg/mL and 0.31 µg/mL, respectively, while at both 316 nm and 330 nm, the LOD and LOQ were 0.12 µg/mL and 0.36 µg/mL, respectively. The accuracy and precision were confirmed using a standard addition method conducted in triplicate at three concentration levels. Consequently, the mean recovery values ranged from 98.40–102.03% at 277 nm, 97.97–102.02% at 316 nm, and 97.76–102.35% at 330 nm, while the repeatability and reproducibility (expressed as RSD%) were below the maximum acceptable set by Horwitz criterion¹ (2.39%). Using classical spectroscopy, the best repeatability was observed at 277 nm at a concentration of 6 µg/mL (0.151%) and the best reproducibility was observed at 9 µg/mL (0.630%). The CIP concentration in the formulation, with expanded measurement uncertainty (MU), was estimated at 3.00 ± 0.07 mg/mL. Using the derivative signal ${}^1D_{267}$, the best repeatability and reproducibility were measured at 6 µg/mL (0.171% and 0.242%, respectively), estimating the CIP concentration with MU at 3.06 ± 0.05 mg/mL. Besides its simplicity, speed, accuracy, and precision, according to the Analytical GREENness calculator², and with an obtained coefficient of 0.82, this method is environmentally friendly and suitable for routine analysis of CIP in eye/ear drop formulations.

Keywords: ciprofloxacin, UV/Vis spectrophotometry, derivative spectrophotometry, validation, quantitative analysis

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Testing Activated Carbon and Amberlite XAD-2 as Sorbents for Passive Sampling of Organochlorine Compounds in Water

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Organochlorine compounds are persistent pollutants that accumulate in water and pose risks to both ecosystems and human health. Therefore, monitoring of these compounds is of great importance, which encourages the development of new methods for their analysis. Within this research, two sorbents, activated carbon and Amberlite XAD-2, were tested for passive sampling in the analysis of organochlorine compounds in water. The sorbents, enclosed in nylon membranes, were exposed to water containing 24 organochlorine pesticides and polychlorinated biphenyls, at time intervals ranging from 2 hours to 14 days, in order to evaluate their ability to retain the target compounds. After exposure, the retained compounds were extracted and analyzed by gas chromatography coupled with electron capture detection. The mass balance was determined for each compound, as well as the time for the passive sampler to reach equilibrium, which ranged from 3 to 10 days for activated carbon, and from 3 to 14 days for Amberlite XAD-2. This study showed that activated carbon and Amberlite XAD-2 are suitable as sorbents for passive sampling of selected organochlorine pesticides and polychlorinated biphenyls, including α -HCH, β -HCH, γ -HCH, *trans*- and *cis*-heptachlor, dieldrin, endrin, α -endosulfan and PCB 52 - indicating their potential applicability for monitoring these compounds in aquatic environment.

Keywords: passive sampler, sorbents, activated carbon, Amberlite XAD-2, organochlorine pesticides, polychlorinated biphenyls, sorbent extraction, GC-ECD.

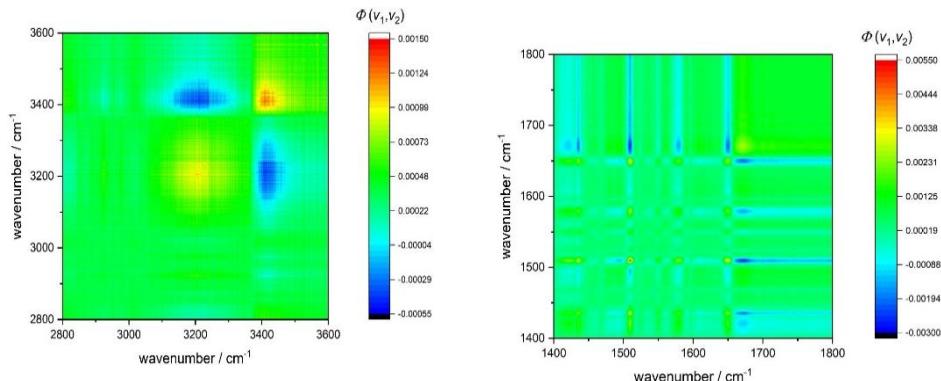
Monitoring Phase Transformation of Pharmaceutical Crystals Using Two-Dimensional Infrared Correlation Spectroscopy

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Temperature-driven phase transformations in crystalline materials play a critical role in determining their stability and functional properties. Two-dimensional infrared correlation spectroscopy (2D-IRCOS) offers a powerful tool for probing these transformations with enhanced spectral resolution. By applying controlled thermal perturbations, synchronous and asynchronous correlation maps were constructed to resolve overlapping vibrational modes and to reveal sequential structural changes hidden in conventional one-dimensional IR spectra. This analysis provides direct insights into the molecular mechanisms underlying polymorphic transitions, including the reorganization of intermolecular interactions and lattice dynamics.



Keywords: Phase transitions, solid materials, two-dimensional correlation spectroscopy, temperature effects, vibrational modes, structural analysis.

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Typical Contaminations Found During Isolation and Growing of Purple Phototrophic Bacteria

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Purple phototrophic bacteria (PPB) are widely studied for their diverse metabolic capabilities and applications in biotechnology³. However, successful isolation and cultivation of PPB are frequently hindered by contamination from various microorganisms. Typical contaminants include fast-growing heterotrophic bacteria such as *Pseudomonas* spp. and *Bacillus* spp., which outcompete PPB in nutrient-rich media¹. Fungal contaminants, especially yeast and molds, also pose challenges during prolonged cultivation². Additionally, phototrophic green sulfur bacteria and cyanobacteria may co-isolate due to overlapping ecological niches, complicating purity assessment⁴. Contamination origins are often linked to sample sources, handling procedures, and media composition. During the research with PPB, the most common contaminants that were encountered were yeasts, molds and *Bacillus* spp. The reasons and contributing factors for this are: environmental conditions, increased factors due to the ongoing laboratory work with the contaminants and their resilience. To minimize the contamination, selective culture media have been used designed to suppress contaminating organisms, with strict adherence to sterile techniques during sampling and cultivation and optimized incubation conditions that favor PPB growth while inhibiting contaminants, such as the use of infrared light, suitable pH and carbon source.

Keywords: purple phototrophic bacteria, contamination, isolation

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The Digital Signature of Metabolites: AI-Powered Biomarker Discovery

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Metabolites are low-molecular-weight chemical compounds within cells, which together constitute the metabolome¹. Metabolomic studies provide a near-real-time view of the phenotype. The resulting biomarker candidates show promise in personalized medicine, early detection, drug discovery and treatment-response monitoring.

However, metabolomic datasets are typically large and complex. Therefore, artificial intelligence (AI) has become an essential tool to obtain reliable, generalizable digital signatures in the analysis of metabolite patterns that reflect various biological states². As a branch of AI, machine learning facilitates detection of metabolic patterns, feature selection, visualization, and the extraction of non-linear relationships from various metabolomic datasets. Although the field of metabolomics and AI-driven biomarker discovery is rapidly growing, several challenges remain, including the high dimensionality of data, batch effects, and limited sample sizes³. These challenges underscore the importance of interdisciplinary collaboration across diverse fields.

This study outlines how AI-driven data mining plays a pivotal role in biomarker identification and in improving clinical relevance of metabolomics. We aim to provide a concise overview of emerging AI methodologies and improvements in metabolic applications enabled by AI-based data processing.

Keywords: metabolomics, artificial intelligence, digital signature, machine learning, biomarker

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Theoretical Basis for Neuroprotective Potential of Intranasal Propolis by Using Sufficiently High Concentrations of Galangin

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The brain is susceptible to oxidative stress due to its high oxygen consumption and rich lipid content. Galangin is not just Cu(II) chelator (by Fenton-like reaction), but it is also a potent antioxidant, scavenger of reactive oxygen species and reactive nitrogen species, thus reducing oxidative damage to neurons, DNA, proteins, and lipids, which is crucial in neurodegenerative diseases and brain injuries^{1,2}. Studies have confirmed the existence of galangin derivatives in propolis, with dose-dependent antioxidant activity³. Enhancing galangin's ability to reach the brain is a challenge due to the blood-brain barrier (BBB) selectivity. The nanotechnology-based approaches to enhance galangin's brain delivery using liposomes, polymeric nanoparticles and nano-suspensions are very popular. Also there are some drug designs for improving the solubility or can be conjugated to galangin by taking over natural transport systems at the BBB which bind to specific receptors on the surface of brain endothelial cells. Invasive methods are possible, however, here it is proposed the most non-invasive approach by intranasal delivery of galangin (the nose-to-brain pathway). The commercial propolis sprays are inadequate because of low concentrations of galangin, however, that can be optimized in pharmacokinetic studies to determine the galangin concentration that reaches the brain in therapeutically relevant concentrations.

Keywords: antioxidant, neuroinflammation, bioavailability, nanosuspension.

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Understanding Hg(II) Removal onto Natural and Modified Zeolite Through Adsorption Isotherm Modeling

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This research focuses on the possibility of using natural zeolite and its modified form for the remediation of mercury-contaminated water systems as well as elucidating the sorption mechanism. For this purpose, natural zeolite clinoptilolite (NZ) originating from the Vranjska Banja deposit, Serbia, as well as its modified form (MZ) was used. Modification of 1 g of NZ was carried out with 50 mL of 1 mol/L $\text{Fe}(\text{NO}_3)_3 \times 9\text{H}_2\text{O}$ for 2 h at 100 °C, and with 10 mL of 1 mol/L $\text{Na}_2\text{S} \times 9\text{H}_2\text{O}$ for 4 h at 150 °C. Physico-chemical characterization of the MZ confirmed successful coating of the starting material with iron sulfide species, since the iron content increased 2.5 times and sulfur by as much as 12 times. Sorption of Hg(II) onto NZ and MZ was carried out under predefined optimal conditions (pH ≈ 2, solid-to-liquid ratio of 10 g/L, and contact time of 24 h) over a wide concentration range of aqueous Hg(II) solutions (0.461–14.099 mmol/L). The maximum sorption capacity of Hg(II) was determined to be 0.288 mmol/g for NZ and 0.996 mmol/g for MZ. The 3.5-fold higher sorption capacity of MZ compared to NZ is a direct result of the modification. Specifically, the stabilization of sulfur in the form of iron sulfide species enhances the sorption capacity of MZ, since sulfur exhibits a strong affinity for Hg(II), consistent with the hard and soft acids and bases (HSAB) theory. Based on the Temkin and Dubinin-Radushkevich isotherm models, the sorption of Hg(II) onto NZ is predominantly physical in nature, whereas the sorption onto MZ occurs primarily through chemisorption and/or ion exchange mechanisms. Ultimately, MZ exhibited a significantly higher sorption capacity for Hg(II) compared to NZ, justifying the modification process. These results indicate that MZ holds strong potential as a sorbent for the remediation of mercury-contaminated aquatic environments.

Keywords: mercury, natural zeolite; modified zeolite, adsorption isotherm, modeling



Iron-Mordenite-Catalyzed Benzene Hydroxylation: Stability via DLS and FMR

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Selective hydroxylation of benzene to phenol remains a challenging reaction in green chemistry. In this work, liquid-phase hydroxylation of benzene with H₂O₂ over iron-containing mordenite was studied using dynamic light scattering (DLS) and ferromagnetic resonance (FMR) techniques to assess catalyst stability and structural changes under reaction conditions. Iron-modified mordenite samples were prepared by impregnation of H-mordenite with Fe(III) and Fe(II) salts, followed by washing, drying, and milling to ~1 μm. DLS measurements revealed a significant increase in particle size during reaction (from ~1.8 to 2.6 μm at 333 K in 6 h), indicating aggregation of iron-containing mordenite particles. FMR spectra showed only minor shifts in resonance parameters, suggesting that the main part of iron oxide species remained stabilized within the mordenite framework. The catalytic activity decreased over time due to surface blocking by reaction products but was almost fully restored after ultrasonic treatment (26 kHz, 10 min). Thermodynamic calculations ($\Delta G^\circ \approx -293$ to -289 kJ·mol⁻¹) confirmed the feasibility of the benzene hydroxylation process, while the reaction yields were limited by kinetic factors. Our results demonstrate that nanosized iron species in mordenite are responsible for H₂O₂ activation and that ultrasound treatment is an effective method for regenerating catalyst activity, highlighting a promising approach for sustainable phenol production.

Keywords: benzene hydroxylation, iron-mordenite, hydrogen peroxide, DLS, FMR



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SP – 45

Origami-Structured Triboelectric Nanogenerator for Efficient Energy Harvesting from Human Motion in Metro Stations

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With the growing demand for sustainable and decentralized power sources to support the next generation of portable electronics and Internet of Things (IoT) devices, triboelectric nanogenerators (TENGs) have emerged as promising candidates for biomechanical energy harvesting¹. In this study, we present the design and characterization of an origami-structured TENG fabricated using nylon and polysiloxane, selected for their complementary positions in the triboelectric series. The TENG was constructed using three layers of each material, each with dimensions of 5×5 cm, arranged to maximize contact area and mechanical deformation during operation.

Experimental evaluations were conducted under external mechanical stimulation using human hand tapping to mimic realistic biomechanical interactions. The device exhibited a maximum open-circuit voltage of 110 V and a short-circuit current of 11 μ A, resulting in an output power of approximately 1.2 mW. These results underscore the potential of the proposed TENG for effective conversion of low-frequency biomechanical energy into electrical energy. The origami-inspired structure significantly contributes to the device's flexibility, resilience, and output performance, making it highly suitable for dynamic, high-traffic environments.

In conclusion, the origami-structured nylon/polysiloxane-based TENG represents a viable and efficient strategy for biomechanical energy harvesting, offering new avenues for powering low-energy devices within the broader scope of sustainable urban development and smart city applications.

Keywords: nylon, polysiloxane, TENG, energy harvesting system, human motion

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Alumina-Based Ni–Fe Catalysts for CO₂ Reforming: Toward Efficient Carbon Utilization

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Nickel–iron catalysts supported on alumina are promising systems for the dry reforming of methane (DRM), combining high activity with relatively low cost and improved resistance to carbon deposition ^{1,2}. In this work, the structural evolution of Ni–Fe/Al₂O₃ catalysts was studied under DRM conditions using SEM–EDX, XRD, and ferromagnetic resonance (FMR). Calcination produced NiO and Fe₂O₃/Fe₃O₄, while reduction yielded metallic Ni, Fe, and Ni–Fe alloys. Strong metal–support interactions led to spinel phases (NiAl₂O₄, FeAl₂O₄), acting as reservoirs for active metals. Under DRM conditions (700–900°C), Ni–Fe alloys dominated, with spinel stabilizing the catalyst. Dynamic redox cycles between Fe²⁺/Fe³⁺ enhance oxygen mobility and carbon gasification. At 700–900°C (typical DRM conditions), equilibrium favors Ni–Fe alloys + residual spinel phases. Ni–Fe alloys are catalytically active, while Fe-containing oxides act as oxygen carriers, suppressing coke accumulation. Ni provides high intrinsic activity for CH₄ activation; Fe dilutes Ni assemblies, reducing coking. Balanced H₂/CO ratios (~1.0) are achievable, but Fe-rich alloys can promote the Boudouard reaction (2CO→C+CO₂). Fe alloying and the formation of partially reducible spinel phases increase resistance to sintering and carbon deposition. These findings highlight the importance of balancing Ni–Fe alloy phases and spinel structures for long-term catalyst stability and efficient DRM performance.

Keywords: Ni–Fe/Al₂O₃; CO₂; CH₄; SEM/EDS; XRD; EPR; DRM.

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The Process of Charging of the Furnaces in R.Ž. Topilnica j.s.c-Skopje

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Furnace charging is a continuous process during the operation of the furnaces. The level of the charge in the bunkers of the electric furnaces in R.Ž. Topilnica j.s.c-Skopje is kept at a minimum of 1/2. Only in special cases is a lower level of the charge in the bunkers allowed, i.e. 1/3 (during the process of technological adjustments of the furnace, before a planned shutdown of the furnace, etc.). Care of the furnace should always be taken about the level of the charge being placed, even when there is a difficult supply, and the furnace power should be reduced in a timely manner. The furnace must not operate when the bunkers are in the smoking process. In such cases, the furnace is turned off and it stands still until it is satisfied with the required batch. The flow of the charge through the charge pipes should be continuous, i.e. there should be no clogged charge pipes, which would disrupt uniform charging, which in turn could lead to other consequences. In the event of a clogged central charge pipe or two or more adjacent auxiliary charge pipes, the furnace is immediately shut down and the necessary measures are taken to unclog the pipes. Also, prolonged operation with one of the auxiliary charge pipes plugged must not be allowed. During the electrode measurement process, the charge supply to the furnace is interrupted by closing the shutters for a period of 2 hours before the furnace piercing process begins. Until the measurement process is performed, the furnace operates at a reduced power of 15 MW. After the measurement is completed, the furnace is not turned on until its interior has been checked (for water leaks), and only then is the furnace charged. Clearly, before the charging process is carried out, a coke correction is placed for better contact. Only after the charging process is completed, the furnace is turned on again, whereby the load on it should be gradual and the normal power of the furnace should be achieved only after 1 hour. In the event that the charge level in the furnace is very low during the electrode measurement, the furnace must not be charged all at once, but in 2 times, with the time interval between one charge and the other being at least 1 hour. During this interval, the furnace operates at a reduced power of 15-18 MW. An improvement could be to replace the chemical quality of the ores (magnetite or siderite) with limonite ore used in the production process, i.e. to make them more easily meltable and have a better granulometric composition. This facilitates the melting process and reduces electricity consumption.

Keywords: Pipes, electric furnaces, bunkers, coke, water leak, reduced power

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Cytotoxic Evaluation of 2-MNQ and 2-HNQ on HepG2 Cells Using the MTT Assay

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The naturally occurring naphthoquinones, 2-methoxy-1,4-naphthoquinone (2-MNQ) and 2-hydroxy-1,4-naphthoquinone (2-HNQ) are found to have potential cytotoxic effect towards tumor cells. Therefore in this study, the MTT assay, a key technique for assessing cell viability², was used to evaluate the effects of 2-MNQ and 2-HNQ on HepG2 cells, a human hepatocyte-derived cell line¹. HepG2 cells were exposed to 0 or 2-MNQ or 2-HNQ in concentration range 0.1 to 100 μ M for 24 h. MTT (0.5 mg/mL) was then added, and after 3 h incubation, formazan crystals were dissolved in DMSO. Quantification of formazan, to distinguish inactive from metabolically active cells, was performed at 570 nm using a microplate reader. In the experiments triplicate wells were used, and experiments were repeated three times. The results are shown as mean \pm SEM.

From obtained results the dose-response curves were created and IC₅₀ calculated. 2-MNQ exhibited significant cytotoxicity toward HepG2 cells with IC₅₀: 7.2 \pm 1.6 μ M. On the other hand, 2-HNQ had minimal effect on HepG2 cells (IC₅₀ \geq 100 μ M). These MTT-based findings highlight the potential of 2-MNQ as a liver cancer therapeutic.

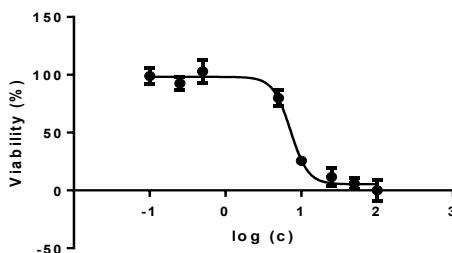


Figure 1. Dose-dependent MNQ inhibition of HepG2 cell viability (%) after 24h treatment. Experimental data were presented as a mean of three separate experiments.

Keywords: 2-MNQ, 2-HNQ, MTT assay, HepG2 cells, cytotoxicity, liver cancer.

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Development of Chirality Sensitive Descriptors for Quantitative Structure-Activity Relationships Modeling

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Chirality is very important property in drug development process. Namely, when quantitative structure-relationship (QSAR) models are developed most of the descriptors used are not *sensitive* to the presence of the chiral atoms. However, often only one of the enantiomers has biological activity. Having this in mind, the development of new chirality sensitive descriptors is very important.

The most often used approach for this purpose is the *fragment rule*. This approach for development of chirality sensitive descriptors is based on calculation of the descriptor from the fragments attached to the chiral atom(s) and, after that, the use of the proper function for calculation of the final descriptors.

Three approaches were used for development of the new descriptors: (1) triple product, (2) vector product and (3) development of the neural networks models based on the descriptors of the fragments attached to the chiral atoms.

The results obtained using the newly proposed approaches were slightly better compared to the existing descriptors capable of distinguishing among chiral molecules.

Keywords: quantitative structure-activity relationship study, QSAR, artificial neural networks, chirality, biological activity.

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SP – 50

Ceramic materials from Industrial and Organic Waste: Technology for Environmental Sustainability

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Industrial waste, generated through manufacturing, industrial and mining activities, represents a significant environmental challenge due to its potential to contaminate local soil and water resources, contaminating the groundwater, as well as lakes, streams, and rivers. A sustainable approach to mitigating these impacts involves the valorization of industrial residues as alternative raw materials for advanced ceramic production. In this study, industrial by-products such as red mud, fly ash and bypass dust (BPD) were investigated in combination with sludge liquids derived from wastewater treatment. The examined and used sludge were obtained using microbial fuel cells (MFCs)—bioelectrochemical systems capable of simultaneously removing organic pollutants from wastewater and generating renewable energy—thus providing an integrated environmental solution. The raw materials were systematically characterized by X-ray fluorescence (XRF), X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) to determine their chemical and mineralogical composition. Behavior during the thermal treatment was also examined by DTA (differential thermal analysis) and DSC (Differential Scanning Calorimetry). Based on these results, a technological protocol was developed for the design of ceramic materials incorporating industrial and organic wastes with low grade clay. Ceramics made from waste reduce the use of primary raw materials, improve waste management and contribute to the circular economy, while providing both ecological and technological benefits.

Keywords: Industrial waste, raw materials, ceramic materials

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