PHYSICAL CHEMISTRY 2026

18th International Conference
on Fundamental and Applied Aspects of
Physical Chemistry

Book of Abstracts

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CONTENT

PHYSICAL CHEMISTRY 2026

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PL *– Plenary lectures*

PL-01

AN UNCONVENTIONAL PATHWAY TO DEVELOP ARTIFICIAL INTELLIGENCE: THE CHEMICAL AI

Pier Luigi Gentili

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Chemical Artificial Intelligence (CAI) is an unconventional paradigm for addressing global challenges. Unlike traditional AI, CAI integrates hardware and software within reactive chemical "wetware" that is maintained far from thermodynamic equilibrium. Inspired by living systems viewed as Information Gathering and Utilizing Systems, CAI seeks to reproduce aspects of biological intelligence, such as sensing, processing, and action. A conceptual knowledge map is presented, spanning molecular, systems, and multiscale chemistry, and encompassing sensors, decision-making units, and effectors. Three main strategies are discussed: chemical logic-based computation, neuromorphic wetware systems, and emerging Quantum AI inspired by quantum phenomena in living matter. By exploiting self-organization and information processing in chemical systems, CAI offers a pathway toward autonomous "chemical robots" and provides new insights into both artificial intelligence and the origin of life.

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PL-02

A BINOMIAL APPROACH TO STOCHASTIC CHEMICAL KINETICS

Gábor Lente

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This contribution introduces a novel approximation technique in the continuous time discrete state approach to chemical kinetics for reactions where a single species is consumed in one or more reactions whose rates can be given based on the concentration of the sole reactant. The essence of the method is that a binomial distribution is assumed to be valid for the molecule numbers of this species, and the probability parameter is obtained as the ratio of the time-dependent concentration and initial concentration, which can be calculated from the analogous model with the deterministic approach. The applicability limits of the approximation are explored by comparing its results with the exact solutions at low initial molecule numbers.

Acknowledgment
The author thanks Prof. János Tóth for insightful discussions.

PL-03

NANOMATERIAL-EMBEDDED MIP SENSORS AND THEIR FUTURE: ADVANCED GREEN STRATEGIES FOR SUSTAINABLE AND RAPID ANALYSIS

Sibel A. Ozkan

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Molecular imprinting technology enables the fabrication of synthetic recognition sites that mimic natural receptors, antibodies, and enzymes. Following template removal, complementary cavities selectively rebind target analytes, providing molecularly imprinted polymers (MIPs) with high affinity, stability, and cost-effective production. However, optimal performance requires careful selection of functional monomers, crosslinkers, and template-to-monomer ratios. Green Analytical Chemistry (GAC) enhances MIP fabrication by replacing hazardous reagents with environmentally benign alternatives and promoting energy-efficient, waste-minimized synthesis. Moreover, integrating hybrid nanomaterials improves sensitivity and selectivity while reducing environmental impact. Consequently, green MIP-based electrochemical sensors provide sustainable, portable, and highly selective platforms for rapid on-site analysis in environmental, biomedical, and food applications.

PL-04

POLARIZED PHASE-SENSITIVE FLUORESCENCE IMAGE CORRELATION SPECTROSCOPY: SIMULTANEOUS CHARACTERIZATION OF LIFETIME HETEROGENEITY AND ROTATIONAL DYNAMICS

Andrew H. A. Clayton

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The spatial and temporal organization of biomolecules is governed by a combination of molecular interactions, aggregation, diffusion, and rotational dynamics. Quantitative determination of these processes in heterogeneous systems remains a significant challenge in biophysical chemistry. Fluorescence lifetime imaging microscopy (FLIM), fluorescence polarization, and image correlation spectroscopy (ICS) each provide complementary information on molecular environment, rotational mobility, and molecular clustering, respectively. In this work, we introduce polarized phase-sensitive fluorescence image correlation spectroscopy (PPS-ICS), a method that combines these orthogonal observables within a single analytical framework. The approach extends phase-sensitive ICS by incorporating polarized excitation and orthogonally polarized fluorescence detection in a frequency-domain FLIM experiment. Images are acquired as a function of detector phase and analyzed using spatial autocorrelation methods to determine phase dependent cluster densities. Simulations

demonstrate that species differing in fluorescence lifetime and rotational correlation time produce characteristic phase-dependent signatures. In particular, slow rotational dynamics reduce polarized fluorescence intensity and introduce additional phase shifts, enabling discrimination of populations that would otherwise be indistinguishable by lifetime measurements alone. A two-state heterogeneous model was investigated as a representative example of molecular populations exhibiting distinct brightness, lifetime, and rotational properties. Application of the method to a model fluorescent bead system demonstrated recovery of cluster densities, relative brightnesses, lifetimes, and rotational correlation times from phase-sensitive image data. The results indicate that PPS ICS provides a route to resolving multiple fluorescent populations and quantifying rotational heterogeneity in complex samples. The methodology offers new opportunities for studying molecular assemblies, oligomerization, membrane domains, and biomolecular condensates, where multiple fluorescent states coexist and conventional imaging approaches often fail to separate underlying dynamic populations.

PL-05

ARTIFICIAL ENZYMES BASED ON METAL OXO-CLUSTERS: FROM DISCRETE SPECIES TO METAL-ORGANIC FRAMEWORKS

Prof. Tatjana N. Parac-Vogt

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Effective catalysts for the controlled transformation of large, complex biomolecules remain rare and challenging to design. In particular, achieving selective protein hydrolysis through non-enzymatic catalysis is difficult, yet critically important for many modern applications in biotechnology and proteomics. In recent years, we have developed a conceptually new strategy for selective protein cleavage by combining the enzyme-like molecular recognition ability of polyoxometalates (POMs), a large family of soluble metal-oxo clusters, with the hydrolytic activity of strong Lewis acid metal cations (Zr, Hf) embedded within the POM framework. Using this approach, selective cleavage has been demonstrated across a range of proteins differing in size, structure, and charge. Building on this, we have shown that metal–organic frameworks (MOFs) based on $\{Zr_6O_8\}$ clusters function as highly effective heterogeneous catalysts for peptide bond hydrolysis in various substrates. These MOFs exhibit excellent catalytic activity across a broad pH range, with significant rate accelerations compared to uncatalyzed reactions. Moreover, UiO-66 Zr-MOF has proven capable of catalyzing both intra- and intermolecular peptide bond formation, notably without inducing epimerization. The potential of metal-oxo clusters as nanozymes for protein hydrolysis has been further illustrated by the discrete $\{Zr_6O_8\}$ cluster, which showed remarkable selectivity in the hydrolysis of myoglobin, cleaving exclusively at six aspartic acid residues out of 154 total residues. Together, these findings highlight that Zr(IV)-oxo cluster-based materials hold strong promise as a new class of dual-function nanozymes, capable of catalyzing both peptide bond hydrolysis and formation.

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PL-06

NETWORK ELECTROCHEMISTRY: SYNCHRONIZATION AND EMERGENT COLLECTIVE DYNAMICS OF ELECTROCHEMICAL REACTIONS

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We investigate the nonlinear dynamics of complex charge-transfer reactions from a network science perspective, with an emphasis on synchronization phenomena induced by migration-current coupling and external feedback. First, we consider microelectrode arrays fabricated by 3D printing and operated in flow cells. In these systems, oscillatory nickel electrodissolution exhibits synchronized current oscillations when migration-current coupling is sufficiently strong. The instantaneous frequencies of the electrode potential oscillations are described using phase models, which enable the extraction of effective coupling networks from experimental data. For two electrodes, strong coupling leads to synchronized behavior at low cell resistance and large distances from the reservoir. For four electrodes arranged as opposing pairs along the flow channel, the theory predicts stronger coupling between the two upstream electrodes, while the coupling strengths among all other electrode pairs remain approximately equal. This network topology is further confirmed in the presence of phase-repulsive external feedback, which produces a nontrivial symmetry-broken three-cluster synchronization state. These findings demonstrate that the three-dimensional placement of electrodes provides new opportunities for studying network structure and nonlinear phenomena in electrochemical systems.

In a parallel line of investigation, we examine synchronization in a fundamentally different interaction topology: a hypernetwork. While many dynamical networks can be described by pairwise interactions, in numerous systems one node can modulate the coupling between two other nodes. Such triadic interactions constitute hyperedges, giving rise to higher-order network structures. To explore these effects experimentally, we implement feedback coupling among oscillatory nickel electrodissolution electrodes. We show that three resonant oscillators do not necessarily exhibit conventional 1:1 synchronization. Instead, they can undergo hyperlocking, a stable phase-triplet locking state arising from higher-order interactions. The experimental observations are quantitatively explained by kinetic modeling and by a second-order phase reduction of coupled Stuart-Landau oscillators. These results reveal a novel synchronization mechanism intrinsic to higher-order interactions and open new avenues for controlling complex dynamical behavior beyond pairwise network frameworks.

A *– Chemical Thermodynamics*

A-01-P

SOLUBILITY IN THE Na_2HPO_4(aq) SYSTEM DETERMINED BY THE ISOPIESTIC METHOD AT 298.15 K

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Phosphate salts, particularly Na_2HPO_4, are widely used in industrial applications ranging from pharmaceuticals to power generation, yet their presence in natural waters presents significant environmental challenges due to eutrophication. A critical evaluation of their thermodynamic properties necessitates accurate solubility data; however, the existing literature for the Na_2HPO_4(aq) system at 298.15 K reveals considerable discrepancies. To address these inconsistencies, this study provides a comprehensive experimental investigation of Na_2HPO_4 solubility using the isopiestic method. After a 30-day equilibration period at 298.15 K, the molality of the saturated Na_2HPO_4 solution was determined to be $m(Na_2HPO_4) = 0.81290 \pm 0.0003$ mol·kg^{-1}. The molalities in isopiestic equilibrium for the reference KCl(aq) solution agreed to within 10^{-3}, confirming that equilibrium was established. This result is in excellent agreement with the value of $m(Na_2HPO_4) = 0.8120$ mol·kg^{-1} reported by Rard and Wolery, validating the experimental methodology and resolving the discrepancies among previously reported literature values.

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B *– Spectroscopy, Molecular Structure, Physical Chemistry of Plasma*

B-01-P

DIRECT SPECTROPHOTOMETRIC DETERMINATION OF α-TOCOPHERYL ACETATE IN PHARMACEUTICAL SOFTGEL CAPSULE

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Fat-soluble vitamins such as vitamin E (mainly α–tocopherol) and its derivative being α–tocopheryl acetate (α–TA) are essential micronutrients that are very significant for health promotion, disease prevention and therapeutic applications. Tocopherols are found in plant foods, but they are also available in commercial products. The purpose of this study is to develop and validate a simple and affordable UV–spectrophotometric method for the determination of α–TA in bulk drug as well as pharmaceutical preparations. The determination of the freely soluble α–TA in ethanol was enforced using the maximum absorbance at 284 nm. Beer's law was obeyed in the α–TA concentration range 19.9–236.4 μg mL^{-1}, with the method sensitivity of 4.7 μg mL^{-1} (the limit of detection, LOD) and 14.4 μg mL^{-1} (the limit of quantification, LOQ). The method applicability to the direct α–TA determination in pharmaceutical preparations (softgel capsules) commercially available on the local market, was demonstrated.

Acknowledgment
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B-02-P

SPECTROFLUORIMETRIC DETERMINATION OF CONTENT OF α– TOCOPHERYL ACETATE IN DIETARY SUPPLEMENTS

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Spectrofluorimetry (SF) and reversed–phase high–performance liquid chromatography (RP–HPLC), used as the reference method, was employed for quantifying α−tocopheryl acetate (α−TA) content in softgel capsules of selected dietary supplements. Based on the obtained fluorescence spectra of standard α−TA solutions in different solvents, ethanol was selected as the solvent for spectrofluorimetric quantification of α−TA in *Natural Wealth*® softgel capsules of dietary supplement. The spectrofluorimetric method was found to be valid for α−TA analysis in the 1.00 –

20.00 μg mL^{-1} linear range. The SF method sensitivity was 0.32 μg mL^{-1} (as limit of detection (LOD)) and 0.97 μg mL^{-1} (as limit of quantification (LOQ)), the accuracy ranging from 97.1 to 103.1% and precision ranging from 2.66 to 4.77%. Obtained validation parameters show that the SF method can be applied for the direct, accurate and precise determination of α–TA content in ethanol solutions and capsules of dietary supplements.

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B-03-P

ELECTRON DENSITY DETERMINATION IN LASER ABLATED PLASMA OF GLASS

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In the present investigation the attempt was made to compare two values of the electron number density in plasma obtained by laser ablation of a glass sample. One value is obtained experimentally by using the Stark-broadened emission profile of the Fe II 261.19 nm line and the other numerically with software developed in our laboratory that solves ionization-recombination equilibriums in plasma assuming the local thermodynamical equilibrium conditions. The numerical results obtained by software are compared with the experimental ones at the temperatures that were previously determined by the Boltzmann plot method for atomic and ionic lines of iron. Relative difference of results is found to be 33% when plasma pressure is assumed constant and equal to 1 bar in numerical analysis, but at higher pressure of 1.6 bar the software obtained the same N_e values as the experiment.

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B-04-P

SPECTROPHOTOMETRIC ASSESSMENT OF MAGNESIUM ION INFLUENCE ON THE PYROGALLOL AUTOXIDATION IN ALKALINE AQUEOUS SOLUTION

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UV-Vis spectrophotometry was used to assess the influence of Mg(II) ions on the pyrogallol autoxidation at pH 9.0 in aqueous solution. Pyrogallol oligomerization/polymerization during autoxidation was evidenced by the changes in the general appearance of UV-Vis spectra with time and steady decrease in *E2/E3* index (A_{250}/A_{365}) values calculated from spectra recorded at various time intervals in both the absence of metal ions and the presence of Mg(II) ions. The important role of Mg(II) ions, especially in the initial phase of pyrogallol autoxidation, was proved by the presence/absence of some typical spectral features and sharpness in *E2/E3* index values decrease with time. UV-Vis spectra recorded after 48 hours of pyrogallol autoxidation in both systems became similar to the spectra of humic acids and enzymatically synthesized poly(pyrogallol). Since poly(pyrogallol) exhibits interesting antioxidant properties, the results of this study may be useful for optimizing its production.

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B-05-P

FORENSIC ANALYSIS OF HEAT-INDUCED STRUCTURAL CHANGES IN PIG BONE USING FTIR AND LIBS SPECTROSCOPY

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Thermally induced changes in pig bone were investigated using Fourier transform infrared spectroscopy (FTIR) and laser-induced breakdown spectroscopy (LIBS). Bone samples were heated at 100 °C and 200 °C for 15 min to examine early thermal alterations of organic and inorganic bone components. LIBS analysis was focused on the spectral region around 250 nm, particularly the C I 247.86 nm and P I 255.33 nm emission lines, while FTIR spectroscopy monitored changes in collagen-, lipid-, and phosphate-related vibrational bands. The most pronounced spectral changes after heating at 200 °C were observed in the 2850–2950 cm^{-1} region corresponding to CH_2 stretching vibrations, indicating thermal reorganization of the organic matrix. Alterations in the amide region confirmed collagen denaturation, whereas phosphate bands of hydroxyapatite remained relatively stable.

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B-06-P

SPECTROFLUORIMETRIC AND MOLECULAR DOCKING STUDY OF BIOMOLECULAR BINDING OF A RUTHENIUM(II)-ARENE COMPLEX CONTAINING 1-PYRENECARBALDEHYDE HYDRAZONE LIGAND

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In this study, the interaction of Ru(II)-arene complex bearing a 1-pyrenecarbaldehyde hydrazone ligand with human serum albumin (HSA) and calf thymus DNA (CT-DNA) was investigated by spectrofluorimetric titration and molecular docking analysis. The complex induced fluorescence quenching of both pure HSA and CT-DNA in the mixture with ethidium bromide, indicating spontaneous binding interactions. Thermodynamic parameters indicated that the binding processes are predominantly entropy-driven and are mainly governed by hydrophobic interactions. Molecular docking calculations confirmed favorable binding of the complex near the Trp214 residue of HSA and within the DNA intercalation region. Good agreement between theoretical and experimental binding energies additionally validated the applied docking protocol and supported the proposed interaction mechanisms.

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B-07-P

THE EFFECT OF COORDINATED CHROMATE ION ON THE HSA BINDING AFFINITY OF [PENTAAMMINECHROMATOCOBALT(III)] COMPLEXES

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The binding affinity of three Co(III) complexes, $[Co(NH_3)_5CrO_4]Cl$ (**1**), $[Co(NH_3)_5CrO_4]_2CrO_4$ (**2**), and $[Co(NH_3)_5Cl]Cl_2$ (**3**), toward human serum albumin (HSA) was investigated using spectrofluorimetric titrations and molecular docking studies. All complexes induced fluorescence

quenching of HSA in the temperature range 300–310 K, indicating spontaneous binding in the vicinity of Trp214 within the FA7 binding site. Thermodynamic parameters indicated that electrostatic interactions and hydrogen bonding primarily stabilize the formed complexes. Molecular docking calculations confirmed spontaneous binding and revealed distinct interaction mechanisms that depend on the coordinated ligand and the overall charge of the complexes. The highest binding affinity was observed for the chromate-containing complex **1**, demonstrating that coordinated chromate ions significantly influence HSA binding behavior.

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B-08-SL

SPATIAL MAPPING OF QUANTITATIVE MOLECULAR INFORMATION VIA MASSIVELY PARALLEL FLUORESCENCE CORRELATION SPECTROSCOPY

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Biomolecules form interconnected reaction networks that regulate cellular functions. Unlike static snapshots of signaling pathways, these molecules dynamically move, interact, and localize in space and time within live cells. Fluorescence Correlation Spectroscopy (FCS) is a powerful fluorescence technique that quantifies molecular concentrations, diffusion and interactions with single-molecule sensitivity and high spatiotemporal resolution. However, conventional FCS is limited by its confocal observation volume, making it difficult to analyze spatially heterogeneous dynamics across cells.

In this lecture, I will introduce massively parallel FCS (mpFCS), a scanning-free confocal microscopy platform we developed [1-4]. A diffractive optical element generates an array of independent excitation foci, while a SPAD camera simultaneously detects fluorescence fluctuations at each spot. This enables quantitative mapping of molecular information across live cells.

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B-09-SL

ORBITAL INTERACTIONS IN CATION-π COMPLEXES OF ORGANOMETALLIC SANDWICH COMPOUNDS – THE IMPORTANCE OF INTRA-FRAGMENT POLARIZATIONS

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Cation-π interactions, primarily those involving aromatic rings, are among the strongest noncovalent interactions and they are essential to many chemical and biological processes [1]. Our recent research showed that aromatic rings can form significantly stronger cation-π interactions when coordinated to transition metals within organometallic sandwich compounds [2].

In order to study the nature of cation-π interactions of organometallic sandwich compounds, the ETS-NOCV (Extended Transiton State – Natural Orbitals for Chemical Valence) methodology was applied [3]. This method enables the decomposition of total interaction energy into physically meaningful components, with the special emphasis on polarization effects, which can be divided into individual orbital interactions and visualized accordingly.

The ETS-NOCV methodology shows that the dominant energy component in cation-π interactions is polarization, especially with smaller cations of more positive charge, and that it is the primary reason for stronger interactions of aromatic rings coordinated to transition metals. Surpsisingly, individial NOCV pairs, that showcase specific orbital interactions responsible for polarization effects, indicate that charge transfer effects are more dominant for cation-π interactions of uncoordinated benzene. However, sandwich compounds suffer from geometry changes duging the formation of cation-π complexes, which induce substantial intra-fragment polarizations, giving additional orbital contributions that provide further stabilization in cation-π interactions of sandwich compounds.

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C *– Kinetics, Catalysis*

C-01-SL

I_2O PREPARATION, VOLATILITY AND POTENTIAL ATMOSPHERIC ROLE

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Diiodine Monoxide (I_2O) is an essential intermediate in the mechanism of the Bray-Liebhafsky oscillating reaction. It is also one of the products of the reactions in solutions of iodine and iodate in concentrated H_2SO_4. We show that it is volatile and can be transferred to the gas phase above these solutions. In the troposphere, it can be formed by the reaction $IO^{\bullet} + I^{\bullet} \rightarrow I_2O$. This formation could play a role in atmospheric chemistry.

C-02-SL

KINETIC STUDY OF Ce(IV)-CATALYZED PHOTOCHEMICAL WATER SPLITTING IN ACIDIC MEDIA

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Photochemical water splitting offers a promising strategy for converting solar energy into hydrogen, which is a sustainable alternative to fossil fuels. The homogeneous Ce(III)/Ce(IV) redox system represents one of the earliest photocatalytic cycles capable of driving the oxidation and reduction half-reactions of water. In the present work, the photochemical oxidation of water by Ce(IV) was investigated in various acids. UV–Vis diode array spectroscopy was employed to monitor the photoreduction of Ce(IV) under continuous irradiation, while oxygen evolution was followed in a PhotoCube photoreactor using an amperometric oxygen sensor and gravimetric measurements. The influence of acid composition and cerium concentration on the reaction kinetics was evaluated. The combined spectroscopic and oxygen evolution measurements provide insight into the mechanism of homogeneous photocatalytic water splitting and the role of cerium speciation in determining the overall reaction rate.

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C-03-O

HYDRODEOXYGENATION OF EUGENOL OVER Ru-CATALYSTS SUPPORTED ON HALLOYSITE NANOTUBES

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An approach is proposed for optimizing the textural and acidic characteristics of halloysite aluminosilicate nanotubes for their use as a catalyst carrier for the hydrodeoxygenation of lignocellulosic bio-oil components. It was found that treatment with a 6 M hydrochloric acid solution for 12 hours increases the inner cavity diameter of the nanotubes (24.7 nm), the specific surface area (154 m^2/g), and the acidity (0.317 mmol/g). Ru-containing catalysts based on both pristine and dealuminated halloysite were synthesized using the microwave-assisted impregnation method. Acid dealumination increased the proportion of active phase nanoparticles localized on the inner surface of halloysite. The ruthenium-containing catalyst synthesized on the basis of dealuminated halloysite exhibits enhanced selectivity toward hydrocarbon formation (up to 77.9%) when using eugenol as a model molecule.

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C-04-P

EFFECT OF COBALT-PALLADIUM CATALYST PRECURSORS MECHANICAL ACTIVATION ON BEHAVIOUR IN CO HYDROGENATION

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Precursors of (10%Co+0.5%Pd)/TiO_2 catalysts obtained by impregnation were activated using high-energy ball milling. Activated precursors were reduced and tested in reaction of CO hydrogenation. Milling reflected on preparatory procedures and on activity and selectivity of materials. Effect of WC instruments application caused increase of catalytic activity. Selectivity was found to reach same levels depending on T_{red} and nature of milling balls (WC and ZrO_2).

C-05-P

THE EFFECT OF TEMPERATURE AND COEXISTING IONS ON ORANGE G DEGRADATION USING COBALT DOPED PSEUDOBOEHMITE CATALYST

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Cobalt-doped pseudoboehmite was used as a catalyst for the Oxone-induced oxidative degradation of the Orange G (OG) dye. Cobalt was introduced into commercial pseudoboehmite using an incipient wetness impregnation method, applying 6 mass% of Co^{2+} relative to the mass of pseudoboehmite. The resulting material was calcined at 500 ºC. The effect of temperature on the dye degradation efficiency was studied, revealing that the degradation rate increases with rising temperature. The results obtained were analyzed using the most common kinetic models, and it was determined that the reaction follows pseudo-first-order kinetics in all instances. The activation energy for the reaction was calculated to be 94.95 kJ mol^{-1}. Additionally, the effect of coexisting cations and anions was also tested. It was determined that the presence of cations (Ca^{2+}, Mg^{2+}, K^{+}, and Na^{+}) inhibited the OG degradation rate. The same was with anions: NO_3^-, SO_4^{2-}, and HCO_3^-, while Cl^- and $H_2PO_4^-$ enhanced the OG degradation.

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C-06-P

EFFECT OF ALCOHOL STRUCTURE ON PHOTOCATALYTIC HYDROGEN PRODUCTION OVER PLATINUM-DECORATED NITROGEN-DOPED TITANATE CATALYST

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Photocatalytic hydrogen production represents a promising strategy for sustainable energy conversion using solar irradiation. Nitrogen-doped titanate catalyst decorated with Pt nanoparticles were synthesized and evaluated for photocatalytic hydrogen production under UV/Vis irradiation. The results showed that the hydrogen production rate strongly depends on the molecular structure of the alcohol. The highest hydrogen production rate was obtained with ethanol (2.2 mmol g^{-1} h^{-1}), followed

by methanol (2.0 mmol g^{-1} h^{-1}) and 2-propanol (1.9 mmol g^{-1} h^{-1}). The observed trend can be explained by differences in adsorption behavior and oxidation kinetics of alcohol molecules on the catalyst surface. Ethanol provides an optimal balance between adsorption strength and oxidation reactivity, facilitating efficient hole scavenging and enhanced charge separation.

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C-07-P

LOW-COBALT-CONTENT Co-Al-CARBON-SMECTITE HYBRID CATALYST FOR HETEROGENEOUS ACTIVATION OF OXONE® IN THE DEGRADATION OF BASIC BLUE 41 IN AQUEOUS SOLUTION

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This study presents a low-cobalt Al-polyoxo-carbon-smectite catalyst for Oxone® activation and degradation of the azo dye Brilliant Blue 41 (BB41). The material was prepared by wet impregnation and treated at 400 °C. Elemental composition (ICP) and textural properties (N_2 physisorption) were analyzed. A Co loading of 10 wt.% was applied; however, only 0.83% was incorporated, indicating preferential binding of cobalt species to the hybrid Al-carbon-smectite structure. The catalyst exhibited a mesoporous structure with higher surface area than the parent material. Oxone®-assisted dye degradation increased from 44% at 25 °C to 96% at 45 °C after 4 h. The process followed pseudo-first-order kinetics with an activation energy of 54.48 kJ mol^{-1}. The lower BB41 degradation, compared with other dyes, is attributed to its stable aromatic heterocyclic structure. These findings demonstrate the promise of low-metal clay-based catalysts for advanced oxidation.

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C-08-P

DESIGN OF Co–Mo/$BiVO_4$ HETEROSTRUCTURES FOR ENHANCED PHOTOCATALYTIC REMOVAL OF ORGANIC POLLUTANTS

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Cobalt and molybdenum co-modified $BiVO_4$ photocatalysts were synthesized via hydrothermal and microwave-assisted methods to investigate the influence of synthesis route on their structural and photocatalytic properties. Photocatalytic activity was evaluated through Methylene Blue degradation under solar and visible light irradiation. The hydrothermally synthesized sample showed superior performance, achieving 55% degradation after 4 h. The enhanced activity is attributed to improved adsorption capacity and number of available active sites. These results highlight the importance of synthesis method in tailoring $BiVO_4$-based photocatalysts for efficient environmental applications.

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C-09-P

OXONE®-ACTIVATED DEGRADATION OF CIPROFLOXACIN USING SYNTHETIC SAPONITES

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Microwave-assisted synthesized saponites were evaluated for the removal of ciprofloxacin through advanced oxidation processes in presence of Oxone®. While pristine Mg–saponite showed higher adsorption capacity (39.69%), the Co-modified sample exhibited superior catalytic performance, achieving up to 88.19% degradation in the presence of Oxone®. Electrochemical analysis revealed that cobalt incorporation enhances electron-transfer kinetics despite a decrease in electrochemically active surface area. The results highlight a clear link between electrochemical properties and catalytic activity, as well as the key role of cobalt in promoting reactive species generation and accelerating the oxidation process.

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C-10-P

IMPACT OF MECHANOCHEMICAL ACTIVATION ON DEXYDROXYLATION KINETICS OF SIVER-DOPED PYROPHYLLITE

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This work examines how mechanical milling duration and silver loading affect the microstructure, morphology, thermal behavior, and dehydroxylation kinetics of pyrophyllite–Ag nanocomposites. Structural and morphological changes were comprehensively evaluated by XRD, FTIR, SEM/EDS, particle size distribution (PSD), and TGA/DTA analyses. The dehydroxylation process was kinetically described using a dispersive kinetics model, which accurately reproduced the experimental conversion profiles. The apparent activation energy varied throughout the reaction, reaching its highest value at the onset, decreasing during the intermediate stage, and increasing again as the reaction approached completion. The findings further demonstrate that the duration of mechanical activation exerts a greater influence on the reaction kinetics than the concentration of $AgNO_3$.

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C-11-P

HYDROISOMERIZATION OF n-HEXADECANE OVER BIZEOLITE SAPO-11+SAPO-31 SUPPORTED Pt CATALYST

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The patterns of formation of SAPO-11/SAPO-31 bizeolite composites were studied depending on the nature of the aluminum source, the type of organic template, temperature, and duration of hydrothermal treatment. XRD analysis showed that aluminum isopropoxide with di-n-propylamine at 200°C for 24 h yields a composite with an optimal AEL/ATO phase ratio. The optimal composite exhibits a total acidity of 540 μmol NH_3/g with only 51 μmol NH_3/g attributed to medium and strong acid sites. In n-hexadecane hydroisomerization at 380°C, the Pt-loaded bizeolite catalyst achieves a

total isomer yield of 73% with 18% multibranched isomers, compared to 67% and 35% for individual Pt/SAPO-31. The obtained material combines the selectivity of the AEL structure with the improved diffusion properties of the ATO phase, making it a promising component of supports for bifunctional hydroisodewaxing catalysts aimed at the production of winter and Arctic diesel fuels.

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C-12-P

KINETIC ANALYSIS OF PARTIAL SUNFLOWER OIL HYDROGENATION OVER MgNi/PERLITE CATALYSTS: EFFECTS OF REDUCTION TEMPERATURE

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A lumped kinetic model with five fatty-acids was used to describe interconversion of linoleic, oleic and stearic species, including cis/trans intermediates. Apparent rate constants were obtained by simplex fitting of experimental concentration profiles and reduced using a relevance criterion ($k_i/k_{max} \geq 1\%$) to identify dominant pathways. The preferred route is direct hydrogenation of cis-linoleic to cis-oleic acid, while high activity alone does not ensure selectivity due to simultaneous trans-isomerization. Precursor with molar ratios Mg:Ni = 0.1 and Ni:SiO_2 = 0.25 was reduced at five temperatures (270, 300, 330, 360 and 390 °C) which strongly influenced the balance between hydrogenation, isomerization and transport effects. Catalysts obtained at reduction interval 330–360 °C showed highest activity, with 360 °C providing the best activity compromise. Kinetic constants thus serve as mechanistic descriptors for catalyst design.

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C-13-SL

EXPERIMENTAL REALIZATION OF THE SIMPLEST REAL CHEMICAL HYPERCYCLE

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The origin of life and the synthesis of autonomous chemical systems rely on mechanisms driving the transition from simple molecular replication to complex, organized networks. A key pathway toward this transition is the hypercycle, a concept introduced by Eigen more than half a century ago.[1] As a higher-order catalytic network, a hypercycle links distinct autocatalytic entities into a cyclic, cooperative hierarchy. In this architecture, the first system's autocatalyst promotes the replication of the second, which in turn accelerates the third, continuing sequentially until the final system closes the loop by catalyzing the first one. This cyclic integration involves nonlinear kinetics and provides a robust mechanism to overcome the error threshold of early genetic systems, thereby preventing mutational meltdown and preserving genetic information. Despite recent advances in complex autocatalytic reaction networks, experimentally realizing a minimal, closed chemical hypercycle remains an elusive goal in systems chemistry. [2-5] Initial experimental approaches relied predominantly on RNA-based networks and ribozyme assemblies. Similarly, recent advances have demonstrated that complex autocatalytic reaction networks can indeed emerge in real chemical systems. Lin and co-workers reported a detailed mechanistic analysis of the methanol-to-hydrocarbons reaction, revealing a dynamically coupled network of autocatalytic pathways.[6] However, despite the presence of multiple interconnected feedback loops, such systems are best described as autocatalytic networks rather than true hypercycles.

Herein, we report the results of our investigations on the tetrathionate-halate reactions coupled successfully as the first direct proof of the existence of a minimal two-membered hypercycle. Both systems were found to be autocatalytic with respect to the corresponding halide ion as products and these ions were experimentally shown to exert a catalytic effect of the other system. This study also serves as a rigorous guiding tool for the chemical community to definitively identify complex systems as true hypercycles and avoid false classifications.

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D *– Nonlinear Dynamics, Oscillatory Reactions, Chaos*

This section is dedicated to
Prof. dr Dragomir Stanisavljev

D-01-SL

FORMATION OF THE TURING PATTERNS IN THE GRAY-SCOTT REACTION-DIFFUSION MODEL INITIALIZED WITH UNIFORM REACTANTS CONCENTRATIONS WITH RANDOM NOISE

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This study examines the robustness of spontaneous Turing pattern formation in the Gray-Scott reaction-diffusion system under varying numerical integration schemes and discretization parameters. Using explicit Euler and fourth-order Runge-Kutta (RK4) methods, we demonstrate that spatio-temporal chaotic and self-replicating patterns emerge from initial uniform concentrations with random noise, confirming that these structures reflect intrinsic model dynamics rather than numerical artifacts. Reduction of the time step size broadens the phase region supporting spontaneous pattern formation, with crescent-shaped parameter domains consistent with prior analyses of perturbed Gray-Scott systems. While finer spatial discretization reduces the pattern-forming region, the parameter neighborhood of (f=0.030, k=0.060) consistently supports pattern emergence across integration methods and resolutions.

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D-02-O

COMPUTER VISION ANALYSIS OF SPATIOTEMPORAL PATTERNS IN THE BELOUSOV-ZHABOTINSKY REACTION UNDER CHEMICAL PERTURBATION

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Glycerol modulates time and pattern of Belousov-Zhabotinsky (BZ) reaction in Petri dish. Patterns in the BZ reaction arise because local chemical oscillations are coupled by diffusion. Using computer vision the spatiotemporal response of a quasi-two-dimensional BZ reaction to a localized glycerol perturbation is quantified. Five consecutive recordings (110.85 min) of experimental (E) and control (K) Petri dishes were processed with rim-excluding masks, a color-opponent score, fixed and frame-

adaptive thresholds, and geometric segmentation. The glycerol was initially localized in E-domain which subsequently evolved from a compact disk/annulus through an elongated oval and directional sector to a nearly uniform pale final state. Fixed-threshold pale coverage reached 50% at 41.98 min, 90% at 63.30 min, and 95% at 72.50 min. Centroid displacement and aspect-ratio changes exclude freely propagating circular-wave behavior. The adaptive black/white partition remains useful as a sensitivity analysis, but it is not an absolute chemical phase fraction. Further analysis are needed to track the specific pattern evolution differences in perturbed and no perturbed state.

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D-03-P

MODELING OSCILLATORY DYNAMICS OF AN AUTOCATALYTIC REACTION MODEL VIA PARAMETRIC NEURAL NETWORKS

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Modeling non-linear chemical oscillators is challenging due to parameter-driven transitions between dynamical states. Conventional integrators must compute the entire transient pathway before reaching a stable limit cycle, making parameter sweeps slow. While Physics-Informed Neural Networks (PINNs) offer an alternative, standard architectures struggle to track these stiff dynamics; trying to resolve both initial transients and stable periodic loops simultaneously leads to training failure. To overcome this, we train a parametric neural network directly on clean periodic orbit data obtained from Poincaré section continuation, completely bypassing transient phases. This data is fed into a multi-output architecture capable of predicting both the concentration profiles of reacting species and the oscillation period for any given parameter. Focused strictly on tracking stable oscillatory regions, our approach provides accurate simulations of long-term temporal dynamics.

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D-04-SL

METABOLIC OSCILLATIONS IN CYANOBACTERIA – A DETAILED MODEL

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Cyanobacteria rely on using two metabolic processes: photosynthesis to produce energy-rich carbohydrates, and fixation of nitrogen to produce nucleic and amino acids. These processes are mutually inhibiting and lead to time-separated oscillatory behavior in a population of single cells or to aggregation of cells into chains, where photosynthesis and nitrogen fixation occur at separate ends and thus are space-separated. Here the focus is on modelling time-separated oscillations observed experimentally in cell suspension of *Cyanothece sp.* Usual dynamical mode is involving alteration of daily light and dark phase but the oscillations are observed even under constant intensity of light when the cells are still viable and their periodic activity is indicated by oxygen release. Interestingly, these oscillations are not controlled by the circadian clock. Rather, they are based on metabolism only and have period much shorter than the circadian rhythms (about 12-17 h). These oscillations have been termed ultradian cycles [1]. Such temporal patterns are a natural way for the cells to survive.

We use the theory of reaction networks to construct a compartmental model of metabolic oscillatory dynamics observed in experiments with photosynthesizing diazotrophic cyanobacteria in a flow-through air-bubbled photobioreactor. The model describes dynamics of component concentrations in two parts of the cell suspension - solution and cellular biomass. Components in the solution are nutrients (CO_2, N_2, O_2), components in the biomass are represented by internal compartments that interact via power law chemical kinetics. The compartments include nutrients inside the cells and functional/structural compartments. The model utilizes experimentally determined biomass growth rate expressed in terms of the Monod kinetics.

The crucial part of modelling is determination of rate coefficients in the power law expressions. We employ the method of constrained stoichiometric analysis [2], which is a combination of stoichiometric network theory and convex linear optimization. The method has been developed in our previous work and successfully used to determine unknown kinetic parameters in oscillatory enzyme reactions. The model is then used to simulate ultradian oscillations under experimental conditions and provides results closely agreeing with the experimentally observed 12-hour ultradian cycles. In addition, bifurcation analysis is used to study dependence of the oscillations on external parameters, namely mass transfer coefficient for gases entering the liquid medium from bubbles and flow rate of the liquid through the reactor.

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D-05-SL

DYNAMICS OF RADIAL PRECIPITATION FRONTS: FROM MICROGRAVITY EXPERIMENTS TO NUMERICAL MODELING

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Radial reaction-diffusion-advection (RDA) fronts sustained by precipitation reactions arise in a variety of natural and industrial processes, including mineralization, reactive transport in porous media, and material synthesis. Their dynamics are strongly influenced by the coupling between chemical reactions and transport phenomena, and can be significantly altered by buoyancy-driven convection resulting from concentration gradients generated across the propagating front.
More generally, chemohydrodynamic instabilities emerge when chemical reactions interact with fluid flows through the generation of density, viscosity, permeability, or surface tension gradients across reactive interfaces. The resulting spatiotemporal patterns can become remarkably intricate due to the nonlinear coupling between chemistry and hydrodynamics, especially when several instability mechanisms, such as buoyancy-driven convection, viscosity contrasts or Marangoni effects, act simultaneously. Understanding the interplay between these mechanisms remains a major challenge in the study of reactive fluid systems.

Under terrestrial conditions, gravity-induced buoyancy strongly affects the dynamics of reactive fronts, adding an additional level of complexity that hides the fundamental mechanisms responsible for pattern formation. In precipitation systems, the interaction between the growing solid phase and the surrounding flow can further modify the local permeability, leading to intricate flow patterns. As a consequence, disentangling the respective roles of buoyancy, dispersion, and interfacial precipitation dynamics from ground-based experiments alone remains challenging. Microgravity environments provide a unique opportunity to suppress buoyancy-driven convection and isolate the intrinsic coupling between transport and precipitation processes, enabling a deeper understanding of the mechanisms governing front morphology and its evolution.

In this work, we focus on radial precipitation fronts generated by the reaction between sodium carbonate (Na_2CO_3) and calcium chloride ($CaCl_2$), which produces solid calcium carbonate ($CaCO_3$) and constitutes a model system for investigating the interplay between reaction, transport, and precipitation under variable gravity conditions and microgravity. Beyond its fundamental interest, this system is relevant to a wide range of applications, including mineral trapping and CO_2 sequestration, polymorph selection, frontal polymerization, and flow-driven chemical garden growth. We combine dedicated microgravity experiments with numerical multiphase simulations to investigate the dynamics of these fronts and to elucidate the mechanisms controlling pattern formation.

D-06-SL

OXIDATION AND REDUCTION FRONTS IN REVERSIBLE REDOX AUTOCATALYTIC NETWORKS

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Autocatalysis is central to the self-organization of chemical and biological systems, underpinning phenomena such as bistability and the emergence of reaction–diffusion fronts. In the rhizosphere, reactive oxygen species are regulated through complex networks of reversible autocatalytic reactions [1–2], but the principles governing their spatiotemporal dynamics are still not fully understood.

Using detailed numerical simulations of a reaction–diffusion model for ROS dynamics that explicitly incorporates redox couples, sodium borohydride, and molecular oxygen, we demonstrate that oxidation-driven autocatalysis constitutes the primary mechanism responsible for the formation of stable reaction–diffusion fronts. These oxidative fronts propagate at constant velocity while preserving a stable spatial profile, in contrast to reduction fronts, which exhibit diffusion-induced broadening that is attenuated by the local oxygen concentration. Furthermore, we show that reversible quadratic autocatalytic cycles, when combined with simple autocatalyst removal and diffusion, are sufficient to reproduce these characteristic front dynamics.

These findings provide broadly applicable insights into the behavior of autocatalytic reaction networks that exhibit spatiotemporal pattern formation.

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D-07-SL

COLLECTIVE DYNAMICS OF SOFT POLYSACCHARIDE MOTORS

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Active matter systems convert supplied energy into directed motion, thereby facilitating selfpropulsion across length scales spanning from the microscopic to the macroscopic regime. Local

interactions among individual constituents can spontaneously generate coherent, emergent collective dynamics. The motility of abiotic particles can be achieved via multiple mechanisms, including Marangoni-driven motion and bubble-induced propulsion. In the former case, the requisite asymmetry originates from spatial gradients in surface tension, whereas in the latter it is imparted by the expulsion of gas bubbles generated through chemical reactions. In this study, we demonstrate that an in situ sol–gel transition of polysaccharide droplets can lead to the formation of a motor that exhibits autonomous self-propulsion.

Upon introduction of a droplet of polysaccharide solution into a bath containing a crosslinking solution, hydrogel beads are generated as the polymer network undergoes gelation. When the surface-active ethanol is incorporated into a chitosan polysaccharide solution, the hydrogel beads formed upon contact with an aqueous sodium hydroxide solution exhibit self-propelled motion at the air–liquid interface. Analogously, droplets of sodium alginate introduced into a calcium chloride solution undergo ionic crosslinking to form calcium alginate hydrogel surfers that similarly display autonomous interfacial self-propulsion. The spatial organization of three or more active surfers in close proximity leads to the emergence of synchronized oscillatory dynamics, arising from intrinsic Marangoni-driven convection in conjunction with capillary-mediated attractive interactions [1,2]. By systematically varying the characteristic size of the active surfers, we identify and classify distinct modes of synchronization [3].

These findings propose a novel strategy for the design of artificial, soft, self-propelled systems that display complex dynamical behavior governed by the interplay between capillary attraction and Marangoni-driven repulsion.

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D-08-SL

RECENT DEVELOPMENTS IN EXPERIMENTAL AND NUMERICAL STUDIES OF THE HYDROGEN PEROXIDE-THIOCYANATE-BASED CHEMICAL OSCILLATORS

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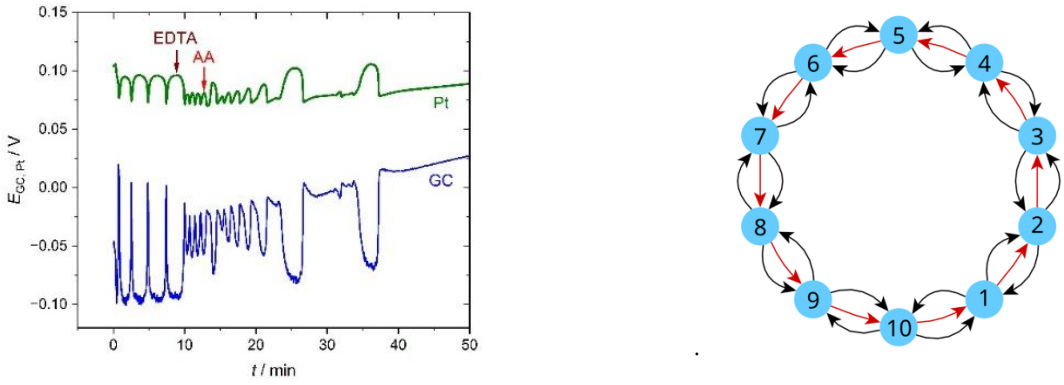
Among the various chemical oscillatory reactions, a special place is occupied by processes occurring in the system: H_2O_2 - SCN^- - OH^- - Cu^{2+}, known as the Orbán-Epstein oscillator [1]. Experimental studies of the influence of various factors on the dynamics of this system have shown i.a., the complex effect of addition of EDTA, causing overproduction of negative feedback $HO_2^{\bullet}$ species [2] and the two-way effect of L-ascorbic acid as both a fast radical scavenger of $HO_2^{\bullet}$ and slower reducing agent of catalytic copper ions (Fig. 1-a) [3].



(a) (b)

Figure 1. (a) Short-time and long-time effect of addition of L-ascorbic acid to the H_2O_2 - SCN^- - OH^- - Cu^{2+} oscillator perturbed by EDTA [3]; (b) The model system of 10 coupled chemical reactors [5] represented as a directed graph designed to study chimera-like states for the simplified 3-variable model of this oscillator [4].

Further studies of the effects of a number of ligands, other than EDTA, also forming thermodynamically stable complexes with copper ions, have shown that this is in general a complex kinetic-thermodynamic issue, requiring numerical modeling for its quantitative analysis and making the chemical oscillator a kind of sensor of the kinetics of copper ion complexation reactions. On the theoretical side, a system consisting of 10 reactors with a simplified 3-variable model of this oscillator [4] was used to study the formation of quasi-chimera states, in which identical coupled oscillators split into subsystems of different dynamic regimes [5]. These studies show the significant continuing research potential of the chemical H_2O_2 – SCN^- - OH^- - Cu^{2+} oscillator and its model mechanisms as an inspiring subject of experimental and theoretical analyses.

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D-09-SL

CONTROLLING REACTION FRONTS WITH HETEROGENEOUS FLOW

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Chemical fronts are localized reaction zones that move through space by reaction and diffusion. They arise across a wide range of settings, from the remediation of pollutants [1] to the propagation of flames [2]. Their properties have most often been studied in rectilinear geometries [3], where fronts advance as planar interfaces. Many real systems, however, involve heterogeneous flows [4,5] and more complex geometries [6,7], where the interplay between reaction, diffusion, and advection governs front propagation.

This talk focuses on a regime where a given flow arrests front motion altogether: the stationary front, held at a fixed location where transport and reaction come into balance. Combining experimental and theoretical approaches, we examine such stationary fronts for two classical reaction schemes: bimolecular A+B→C fronts [8] and autocatalytic fronts [9]. In each case, an imposed flow can hold the reactive zone in place, and its position becomes a controllable property, set by the balance of reaction, diffusion, and the local flow field. Beyond simply arresting a front, the flow can also reshape it, destabilize the reactive interface and select the spatial patterns it forms [10].

By showing that the propagation and spatial organization of chemical fronts can be controlled through flows, this work contributes to the understanding of chemo-hydrodynamic systems. It also points toward strategies for controlling reactive transport, with relevance to environmental, industrial, and biological applications where chemical fronts advance through structured transport networks.

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E *– Electrochemistry*

E-01-O

GO@AuNPS-INTEGRATED MOLECULARLY IMPRINTED ELECTROCHEMICAL SENSOR FOR RAPID AND SELECTIVE ANTIBIOTIC DETECTION

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Ceftazidime (CTZ) is a widely prescribed third-generation cephalosporin, and accurate concentration determination is essential for therapeutic drug monitoring and pharmaceutical quality control. Herein, we developed a molecularly imprinted polymer (MIP)-based electrochemical sensor incorporating a graphene oxide/gold nanoparticle (GO@AuNPs) nanocomposite for ultrasensitive CTZ detection. The GO@AuNPs matrix enhanced electron transfer and increased the active surface area, while the MIP layer, prepared by photopolymerization using trans-3-(3-pyridyl)acrylic acid (3,3-PAA), provided highly selective recognition sites. Under optimized conditions, the sensor exhibited a linear range of 2.50×10^{-13}–3.75×10^{-12} M and an LOD of 5.65×10^{-14} M. It achieved excellent selectivity even in the presence of a 1000-fold excess of interferents. The sensor was successfully applied to serum and pharmaceutical samples, yielding recoveries of 98.61–99.82% and demonstrating its reliability and practical applicability for CTZ analysis.

E-02-P

THE EFFECT OF THE CALCINATION PROCEDURE ON THE ELECTROCHEMICAL RESPONSE OF CARBON–ALUMINA ELECTRODES TO PENDIMETHALIN

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Carbon–alumina composites were synthesised by introducing carbon black into an alumina sol followed by calcination under conventional and flash regimes. The resulting materials were used as modifiers for carbon paste electrodes. The electrochemical behaviour of the modified electrodes was tested in the electroreduction of pendimethalin. The results showed a significant influence of the chosen calcination method on the electrochemical properties of the carbon-alumina-based electrodes.

Acknowledgment
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E-03-P

SQUARE WAVE VOLTAMMETRIC METHOD FOR INVESTIGATION OF GEFITINIB BEHAVIOR AT DNA-MODIFIED GLASSY CARBON ELECTRODE

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Gefitinib (GEF), a tyrosine kinase inhibitor, was investigated for its interaction with double-stranded DNA using a DNA-modified glassy carbon electrode in combination with square-wave voltammetry. The biosensor was incubated in GEF solutions ranging from 5×10^{-6} to 2×10^{-4} M, and changes in the deoxyadenosine (dA) oxidation peak were analyzed. At the lowest GEF concentration, a decrease in dA peak current and a slight shift toward more positive potentials suggested the formation of non-covalent GEF–DNA complexes. In contrast, higher concentrations produced increased peak currents and more pronounced positive potential shifts, indicating DNA conformational rearrangements and structural alterations. These findings demonstrate a concentration-dependent and multifaceted mechanism of GEF–DNA interaction.

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E-04-P

ELECTROCHEMICAL STUDY OF TWO SIRT2 INHIBITORS OXIDATION BEHAVIOR AND INTERACTION WITH DNA

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The electrochemical behavior of SIRT2 inhibitors AGK2 and SirReal2 (SR2) was investigated at a glassy carbon electrode, with emphasis on optimizing conditions for DNA interaction studies. Both compounds exhibited a single irreversible anodic peak below 1.0 V and diffusion-controlled oxidation. Due to limited aqueous solubility, dimethyl sulfoxide (DMSO) was introduced, with 40% (v/v) providing best signal definition for electrochemical behavior studies. Considering its concentration-dependent effect on DNA, interaction studies were performed at 10% (v/v) DMSO using a DNA-modified electrode in acetate buffer (pH 4.6). Interactions were monitored via the change in deoxyadenosine (dA) signal. Both inhibitors caused a concentration-dependent decrease in

dA current accompanied by a positive shift in peak potential, confirming DNA binding, with the strongest effect observed at the lowest concentrations.

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E-05-P

DIFFERENTIAL PUSE VOLTAMMETRIC METHOD FOR INVESTIGATION OF THIOUREA DERIVATIVE OF NAPROXEN INTERACTION WITH HUMAN SERUM ALBUMIN IN THE PRESENCE OF DMSO

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The interaction between a thiourea derivative of naproxen (TDN) and human serum albumin (HSA) was investigated using differential pulse voltammetry (DPV). Measurements were performed in PBS (pH 7.35) containing 30% (v/v) DMSO, ensuring adequate solubility and stable electrochemical response. TDN exhibited two oxidation peaks, with the main peak at ~0.98 V used for analysis. Increasing HSA concentration caused a positive shift in peak potential and a decrease in peak current, indicating complex formation. The fraction of bound TDN was quantified from current changes, revealing that 99.85% of TDN (5×10^{-5} M) binds to HSA (1×10^{-5} M). These results demonstrate a strong affinity of TDN for HSA and confirm the applicability of DPV for studying drug–protein interactions.

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E-06-P

CATALYST FROM RECYCLED CPUs AND BIOMASS FOR SUPERCAPACITORS

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Lemon peel biowaste and recycled CPU leachates were employed as precursors for the synthesis of carbon-based electrocatalysts and energy-storage materials. Chemical activation route used *aqua regia* (AR) solution enriched with metal ions from dissolved CPUs combined with CO_2 physical activation at 800 °C, yielded a series of porous carbons with distinct surface chemistries and morphologies. The resulting materials were evaluated for supercapacitor applications. This materials exhibited significant capacitive behavior. In particular, the AR + CO_2 sample achieved a specific capacitance of ~106 F g^{-1} in acidic media. These results highlight a circular economy strategy contributing to both clean energy generation and sustainable waste management.

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E-07-P

DIELECTRIC BARRIER DISCHARGE OXIDATION OF TETRAHYDROFURAN TO GAMMA-BUTYROLACTONE

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The objective of the present research is to demonstrate the efficiency of gamma-butyrolactone synthesis via tetrahydrofuran oxidation under dielectric barrier discharge conditions. The oxidation was performed at atmospheric pressure using air as an oxidizing agent in a one-barrier 2 mm gap reactor at the frequency of 2000 Hz and impulse amplitude of 8.5 kV without heating or cooling. The products were analyzed using gas chromatograph equipped with Agilent HP-1 column and flame ionization detector. It was established that 6 wt.% of tetrahydrofuran was converted to gamma-butrolactone with the selectivity of 21 wt.% at a tetrahydrofuran residence time of 15 s. The results obtained confirm the viability of discharge-induced oxidation of tetrahydrofuran for its practical application in gamma-butyrolactone production.

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E-08-P

Ni-Fe DOPED GRAPHENE AEROGELS AS EFFICIENT ELECTROCATALYSTS FOR TWO-ELECTRON OXYGEN REDUCTION REACTION

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Electrochemical oxygen reduction reaction (ORR) is essential for sustainable energy conversion and green hydrogen peroxide (H_2O_2) production. In this study, the electrocatalytic performance of graphene aerogels decorated with nickel and iron nanoparticles (Ni_xFe_{100-x}/GA) for oxygen reduction to H_2O_2 was investigated in alkaline medium (1 M KOH). Owing to their 3D porous structure, high specific surface area, low density, and excellent conductivity, this class of materials represents a promising low-cost alternative to Pt-based catalysts. Linear sweep voltammetry confirmed a selective two-electron ORR pathway with the number of exchanged electrons of 2, enabling efficient H_2O_2 generation. The onset potential values for the tested materials are in the range from 0.72 to 0.78 V vs. RHE, and the Tafel slope values are from 107 to 159 mV dec^{-1}. The obtained results indicate the potential application of these materials for the in situ electroproduction of green H_2O_2 in the electro-Fenton process, which is one of the most important technological procedures for wastewater treatment, which avoids environmental pollution.

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E-09-SL

BEYOND NOBLE METALS: HARNESSING MULTIMETALLIC SYNERGY AND MORPHOLOGY FOR EFFICIENT WATER ELECTROLYSIS

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Amid the current global energy crisis, driven by geopolitical conflicts in the Middle East, growing environmental concerns, and continued reliance on fossil fuels, extensive research and innovation are being devoted to the development of clean, sustainable, and renewable energy alternatives. Green hydrogen is increasingly recognized as a promising option for the decarbonization of carbon-intensive industrial processes and sectors. However, green hydrogen production remains economically uncompetitive, with renewable electricity accounting for approximately 60% of its production cost. In addition, the relatively high cost of hydrogen is strongly influenced by the capital and operating costs of electrolyzer and fuel cell technologies. One promising strategy for supporting the transition to a sustainable energy system is the conversion of excess renewable electricity into green hydrogen through the electrolytic splitting of water. Large-scale water electrolysis, however, requires the development of efficient, cost-effective, and durable electrocatalysts for both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Particular attention is therefore focused on platinum-group-metal-free (PGM-free) electrocatalysts that reduce dependence on critical and scarce elements. Replacing Pt-based cathode catalysts and Ir-based anode catalysts remains a major challenge due to their outstanding catalytic activity and long-term stability. In this work, we focus not only on enhancing the intrinsic catalytic activity of electrocatalysts but also on increasing their electrochemically active surface area to provide a high density of accessible active sites for gas evolution. Our approach is based on the design and synthesis of multimetallic electrocatalysts exhibiting strong synergistic interactions and enhanced electron-transfer kinetics, combined with tailored morphologies, including powders, fibers, and hollow micro-/nanostructures. The most promising catalysts are evaluated in both alkaline and acidic electrolytes using a three-electrode configuration with a rotating disk electrode. Their electrochemical performance is systematically assessed by linear sweep voltammetry, cyclic voltammetry, electrochemical impedance spectroscopy, Tafel analysis, electrochemically active surface area determination, and activation energy measurements. The results demonstrate the potential of multimetallic catalysts with tailored composition and engineered morphology as efficient, durable, and economically viable alternatives to conventional noble-metal-based electrocatalysts for water electrolysis.

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E-10-SL

COLLECTIVE MATTER-FIELD DYNAMICS IN WATER UNDER MODERATE HIGH-VOLTAGE ELECTRIC FIELDS

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Understanding the response of water to moderate yet technologically relevant high-voltage electric fields is important for biological systems, water-treatment processes, and interfacial phenomena. In this study, pure water exposed to non-homogeneous electric fields of approximately a million volts per meter is investigated using a free-hanging horizontal electrohydrodynamic bridge. This field

regime is commonly encountered in electrohydrodynamic devices and biological membranes. Spatially resolved Raman spectroscopy reveals mesoscopic signatures in the form of sidebands within the OH-stretching region. In conjunction with QENS, IR emission and ultrafast pump-probe studies, these observations suggest the presence of dynamically ordered water domains exhibiting vibronic coupling. The findings provide new physicochemical insights into electrically stressed water and are consistent with mesoscopic ordering phenomena relevant to applied water systems.

F – Biophysical Chemistry, EPR investigations of Bio-systems

This section is dedicated to
Prof. dr Goran Bačić

F-01-P

SYNTHESIS AND CHARACTERIZATION OF LIPID NANOPARTICLES CONTAINING GFP mRNA

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Lipid nanoparticles (LNP) are currently the most clinically validated platform for mRNA delivery. This study presents a thin-film hydration adaptation of the commercial Moderna LNP formulation, with fluorescently labeled BND-25 cholesterol incorporated for intracellular tracking. Green fluorescent protein (GFP)-encoding mRNA was prepared by *in vitro* transcription from linearized plasmid templates, with uridine fully replaced by N1-methylpseudouridine to improve translation, increase functional stability, and reduce innate immune activation. The hydrodynamic size of empty and mRNA-loaded LNPs was determined by dynamic light scattering (DLS), and membrane fluidity by electron paramagnetic resonance (EPR) spectroscopy with 5-doxyl stearate as spin probe, giving order parameters consistent with stable LNP formation. RNA encapsulation efficiency, measured by the RiboGreen assay, was 82 ± 4.11% (n = 3). Transmission electron microscopy, fluorescence microscopy, and flow cytometry showed time-dependent uptake of LNPs by THP-1 cells over 24 h, partial association of the internalized material with LC3-positive vesicles, and increased green fluorescence in treated cells. These findings demonstrate the feasibility of the thin-film approach for preparing mRNA-loaded LNPs.

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F-02-P

EPR STUDY OF THE RADICAL-SCAVENGING POTENTIAL OF ROOT, STEM, AND LEAF EXTRACTS OF *Arum maculatum*

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Rationale: *Arum maculatum* exhibits a wide range of biological activities, from anti-inflammatory to anticancer. As free radical scavenging is a critical characteristic of compounds with potential therapeutic efficacy, the aim of this work is to evaluate the antioxidant activity of the *A. maculatum* plant extract. **Methods**: In this experiment 50% EtOH extracts of the root, stem and leaf of the *A.*

maculatum were used. Antioxidant activity toward DPPH, hydroxyl and superoxide anion radicals was examined using EPR spectroscopy. **Results and Conclusion**: The highest antioxidant activity was observed in the leaf extract, the lowest in the stem. Extracts of all three parts of the plant showed the highest efficiency for scavenging hydroxyl radicals and the lowest for superoxide radicals. The demonstrated radical-scavenging capacity, particularly against hydroxyl radicals, supports the potential of *A. maculatum* as a promising natural source of antioxidants, significant for further pharmacological investigation.

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F-03-SL

ELECTROCHEMICAL AND FIELD EFFECT TRANSISTOR APTASENSOR FOR REAL-TIME CARCINOEMBRYONIC ANTIGEN DETECTION

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This work presents a novel dual-mode electrochemical (EC) and field-effect transistor (FET) aptasensor based on reduced graphene oxide (rGO) for the rapid, label-free, and highly sensitive detection of carcinoembryonic antigen (CEA), a key cancer biomarker. The sensor integrates an interdigitated electrode architecture, allowing for both EC and FET measurements on a single chip. The FET mode achieves an exceptional limit of detection (LoD) of 60 ag/mL with a response time of 2 minutes, while the EC mode extends the dynamic range up to 1 ng/mL. The aptasensor demonstrates high selectivity and successful detection in saliva samples, showcasing its potential for non-invasive point-of-care diagnostics and cancer treatment monitoring.

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F-04-SL

NEW ADVANCEMENTS IN MODELLING OF INHOMOGENEOUS PHYSIOLOGICAL STRUCTURES AND ASSOCIATED TRANSPORT PROCESSES OF CLINICAL SIGNIFICANCE

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Modelling for Digital Twins for Physiology (or more precisely Precision Medicine), garnered significant attention in recent years. One of our research projects that developed such Digital Twin was exploring the transdermal transport of fentanyl for oncology patients who need personalized dosing, while using standardized skin patches. The main task here is to estimate the quantity of molecules that pass all the skin layers and reach the circulation, from the patch homogeneous gel reservoar, as clinicians warned that the majority of patients are overdosed with this potentially fatal substance. As we experienced before, like in standard approach to electrical signal analytics that uses a mechanistic (reductionistic) approach, that neglects the fractal structure and processes, as well as unpredictable complex systems dynamics in physiology, this path to modelling was using oversimplification, too. That approach was demonstrated before to lead to misinterpretation. We analyzed all the previous knowledge applied (pharmacokinetics and pharmacodynamics) and scrutinized existing model that was based on diffusion processes, with presumption that skin is a homogeneous medium. Then we developed fractal description of that physiological reality, tortuous possible paths included, and included also inertial processes and fractional calculus to improve that initial modelling framework. We demonstrated that instead of Fick's second law, we are witnessing Anomalous diffusion. Besides simulation and comparison of several theoretical frameworks to accurately describe what is physiological reality, we showed that in comparison with timeline of accumulation of molecules that entered via skin, known from plasma concentrations from volunteers (datashare from another laboratory), existing diffusion based model is an oversimplification that should be replaced with anomalous diffusion approach. In continuation of our research, beside anomalous diffusion, we also explored important boundary conditions and some memory features of an inhomogeneous medium, important for potential clinical decisions. This lecture is in a way an overview of our prior work, that examines possible advancements of modelling improvement for physiological processes, by taking in account physiological complexity and complex systems dynamics, to avoid misinterpretations and allow for real precision medicine recommendations.

G *– Organic Physical Chemistry*

G-01-P

PHYSICOCHEMICAL PROPERTIES OF HYDROXYPROPYL METHYLCELLULOSE - A COMPONENT OF BUILDING MIXTURES

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We have developed a laboratory method of synthesis of hydroxypropyl methylcellulose (meilose) from α-cellulose (cotton). The glass transition temperatures of synthesized meilose and meilose produced in Germany were determined using differential scanning calorimetry. We have established two glass transition temperatures in these samples. Thermogravimetric studies made it possible to establish the temperatures of dehydration of sorption water and thermal decomposition. The functional composition of meilose samples was studied using IR spectroscopy.

H *– Material Science*

H-01-O

THERMODIFFUSION AND REPELLENT ACTIVITY OF DERIVATIVES OF ALKYL BUTYL ACETYL AMINOPROPIONATE

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Vector-borne diseases are a major public health issue. Arthropods and rodents are vectors of hundreds of pathogens that cause millions of deaths every year. Insecticides, acaricides and repellents are used to prevent vector-borne diseases. In this study, we propose a new control-released material with repellent activity against ixodid ticks. The active substances used were alkyl butyl acetyl aminopropionates. Thin films containing repellents based on hydroxypropylcellulose were produced. The thermodiffusion of the repellent was studied at different temperatures. The impact of temperature and repellent concentration to the diffusion was determined.

H-02-O

GRAPHENE OXIDE-BASED HUMIDITY SENSORS MODIFIED BY CARBON ION BEAM IRRADIATION

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Graphene oxide (GO)-based materials have attracted significant attention for humidity sensing applications due to their tunable surface chemistry and strong dependence of electrical properties on moisture content. In this work, thin films of GO and GO-based composites containing 15 wt.% of tungstophosphoric acid (WPA), cobalt ferrite (CFO) were deposited on interdigital electrodes and irradiated with 2 MeV carbon ions at fluences from 1×10^{13} to 1×10^{15} ions cm^{-2}. Humidity-dependent impedance measurements were performed at 30 °C in the 35–75% RH range using impedance spectroscopy in the 10 Hz–100 kHz range. All samples showed strong dependence of impedance on humidity. GO/WPA 15% irradiated with 1×10^{13} ions cm^{-2} exhibited the most linear response with ~43% impedance decrease, while GO/CFO_HT 15% showed the largest impedance variation (from 3 MΩ to 70 kΩ). The results demonstrate that incorporation of inorganic components into GO matrix and ion beam irradiation provide an effective route for tailoring humidity sensing properties of GO-based nanocomposites.

Acknowledgment
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H-03-O

KEY ASPECTS OF SYNTHESIS AND APPLICATIONS OF COBALT FERRITE NANOPARTICLES

Sonja Jovanović [1], Marija Milićević [1], Zoran Jovanović [1], Danica Bajuk-Bogdanović [2], Melita Tramšek [3], Matjaž Spreitzer [4], and Davide Peddis [1,5,6]

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This work summarizes findings of our recent studies examining the synthesis of cobalt ferrite (CFO), its chemical modification through zinc substitution and surface functionalization. Also, it addresses the impact of such modifications on structural, magnetic and surface properties and diverse applications of CFO nanoparticles. We demonstrate the potential of the solvothermal synthesis for precise control of nanoparticle size and morphology, while zinc doping, in a one-pot and single-step approach, provides a powerful strategy for tuning magnetic properties without altering particle size or morphology. Key results show that Zn^{2+} substitution changes saturation magnetization, coercivity, and blocking temperature through cation redistribution and anisotropy reduction. Surface functionalization, particularly oleic acid capping and ligand exchange with dihydrocaffeic acid, enable versatile applications of CFO ranging from electrochemical sensing to magnetic resonance imaging and drug delivery.

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H-04-P

GAMMA RADIATION SYNTHESIS OF THERMOSENSITIVE P(OPGMA/IA) HYDROGELS: EFFECT OF COMONOMER COMPOSITION ON SWELLING AND GENOTOXICITY

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Copolymeric hydrogels based on oligo(propylene glycol) methacrylate (OPGMA) and itaconic acid (IA) were successfully synthesized via gamma radiation polymerization using varying monomer ratios. Results showed that increasing the content of IA significantly impacted the gel fraction. Higher IA content also enhanced the swelling capacity, suggesting improved hydrophilicity and water uptake behavior. Importantly, the volume phase transition temperature (VPTT) shifted toward physiological temperature ranges, indicating potential suitability for biomedical and stimuli-responsive applications. Genotoxicity assessment indicated satisfactory biocompatibility of the synthesized hydrogels, with no clear IA concentration-dependent effect. These results highlight their tunable properties and support potential biomedical applications, while indicating the need for further evaluation to confirm safety.

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H-05-P

THERMORESPONSIVE PNIPAM HYDROGELS SYNTHESIZED BY LOW-DOSE GAMMA RADIATION: EFFECT OF CROSSLINKER ON SWELLING AND MORPHOLOGY

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This study presents the characterization of three samples of poly(N-isopropylacrylamide) (PNiPAM) hydrogels synthesized using a low irradiation dose (5 kGy). The hydrogels were prepared without a crosslinker and with two chemically different crosslinkers (methacrylate- and acrylamide-based) to evaluate the influence on network structure. The materials were analyzed by determining gel content and swelling behavior. Dynamic swelling measurements were performed at temperatures below, near, and above the volume phase transition temperature (VPTT) to assess swelling kinetics and determine the time to reach the swelling equilibrium. Morphology was examined by scanning electron

microscopy (SEM) for qualitative comparison of structural differences. The results highlight the effect of crosslinker presence and type on hydrogel properties.

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H-06-P

TUNING PNIPAM HYDROGEL PROPERTIES THROUGH GAMMA IRRADIATION DOSE: GEL FRACTION, SWELLING, AND BIOCOMPATIBILITY

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This study reports the characterization of four series of poly(N-isopropylacrylamide) (PNiPAM) hydrogels synthesized via gamma irradiation at doses of 5, 10, 15, and 25 kGy in aqueous media without a crosslinker. The hydrogels were evaluated in terms of gel fraction and swelling behavior, showing gel fractions increasing from approximately 89% to 99% with increasing irradiation dose, while equilibrium swelling ratios varied significantly with temperature and irradiation conditions (e.g., from 20 g/g for samples irradiated at 25 kGy to 50 g/g for samples irradiated at 5 kGy, measured at 10 °C). Their biocompatibility was assessed using a cell viability assay, with all samples maintaining high cell viability above ~90%, indicating low cytotoxicity. The results demonstrate a clear influence of irradiation dose on physicochemical properties and performance, while all samples exhibited favorable biocompatibility.

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H-07-P

SYNTHESIS AND CHARACTERIZATION OF BIOCHAR-BASED ADSORBENTS FOR THE REMOVAL OF THE AZO DYES FROM WASTEWATER

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Tartrazine (AY23), a widely used azo dye in food, textile, and cosmetic industries, is an environmental concern due to its persistence and toxicity. In this study, biochar derived from Turkish oak (*Quercus cerris*) sawdust was chemically activated with H_3PO_4, NaOH, and H_2O_2 (4:1 activator:sawdust ratio), carbonized under air-limited conditions, and evaluated for AY23 adsorption from aqueous solution. Among the prepared materials, only the H_3PO_4-activated biochar (denoted as CP) showed significant adsorption efficiency and was therefore further characterized. Scanning electron microscopy (SEM) revealed its morphology, while N_2 physisorption showed a high specific surface area of 1060.8 m^2/g. Batch adsorption experiments demonstrated that AY23 removal depended on the initial dye concentration, and the equilibrium data were best fitted by the Redlich-Peterson and Sips models (R^2 = 0.997). These results highlight CP biochar as a sustainable and effective adsorbent for azo dye removal.

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H-08-P

NOVEL REPELLENT MATERIALS BASED ON DERIVATIVES OF ALKYL BUTYL ACETYL AMINOPROPIONATE

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New repellent materials based on alkyl butyl acetyl aminopropionate from blood-sucking insects were obtained. The synthesis of the 3-(N-butylacetamido)propionic acid was carried out, followed by the production of derivatives of alkyl butyl acetyl aminopropionate. The obtained substances were characterized using infrared spectroscopy, nuclear magnetic resonance spectroscopy and high-performance liquid chromatography with tandem mass spectrometry. Repellent materials based on polyacrylic films contained aluminum oxide sorbent with synthesized compounds were prepared. Studies assessing the biological activity of the composite materials have shown that the repellency coefficient was approximately 90-95% for all synthesized substances, suggesting that the material could serve as an alternative to current mosquito repellents.

H-09-P

PHASE STRUCTURE AND DEFECTS OF BIO- SYNTHESIZED ZrO_2-CeO_2 SYSTEM

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The aim of the present study was to investigate the phase structure and the presence of some defects in phyto-synthesized ZrO_2-CeO_2 composites using lavender extract. The particles were characterized by X-ray diffraction (XRD) and Electron paramagnetic resonance (EPR). The X-ray diffraction patterns of our samples indicate the formation of a predominant solid solution phase. Tetragonal phase was registered in all of the samples. The microstrains were higher in the cases of ZrO_2-CeO_2 (50%) and ZrO_2, indicating lattice distortion due to cation substitution and some defect-induced effects. When the Ce concentration increases above 10 at%, the EPR results reveal a decrease in Zr^{3+} sites and a concomitant increase in Ce^{3+} ions, oxygen vacancies and surface oxygen radicals, indicating enhanced defect density and redox activity.

The ZrO_2-CeO_2 bio-composites could be useful for various applications in several fields in the industry: as catalysts/photocatalysts, gas sensors and corrosion inhibitors in sea water.

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H-10-P

ELECTROCATALYTIC PERFORMANCE OF GREEN-SYNTHESIZED SILVER-POLYPYRROLE NANOCOMPOSITES

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A sustainable green approach for the synthesis of silver-polypyrrole (AgPPy) nanocomposites as highly active oxygen reduction reaction (ORR) electrocatalysts is presented. The Ag nanoparticles, prepared using lemon juice as a reducing and stabilizing agent, were combined with pyrrole via in situ oxidative polymerization, yielding a series of nanocomposites with tunable Ag content, spherical particle size, and surface chemistry. Electrochemical characterization in alkaline media demonstrated that all nanocomposites are active toward ORR, with pronounced differences in electrochemically active surface area, kinetic parameters, and reaction pathways.

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H-11-P

PREPARATION AND CHARACTERIZATION OF CHITOSAN/SURFACTANT-MODIFIED PHILLIPSITE COMPOSITE FOR CONGO RED REMOVAL

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Surfactant-modified zeolites show enhanced affinity toward anionic pollutants; however, their powdered form limits practical application in continuous treatment systems. In this study, surfactant-modified phillipsite (PC200) was immobilized within a chitosan matrix to obtain stable composite beads (Ch-PC200) for Congo red removal. The composite was prepared by incorporating PC200 into a chitosan solution followed by bead formation in NaOH and freeze-drying. ATR-FTIR analysis confirmed the presence of characteristic bands of both components and indicated interactions between chitosan functional groups and modified phillipsite. Preliminary adsorption experiments showed that dye removal increased with adsorbent dosage, reaching 34.9% at 2.5 g L^{-1}. Kinetic experiments revealed rapid initial adsorption followed by slower equilibrium attainment. Both pseudo-first-order and pseudo-second-order models adequately described the experimental data ($R^2 > 0.98$), with calculated adsorption capacities of 6.1 and 7.7 mg g^{-1}, respectively. The results demonstrate the potential of Ch-PC200 as a structurally stable adsorbent for further optimization in dye removal applications.

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H-12-P

EFFECT OF SYNTHESIS METHODS ON UREA-FUNCTIONALIZED CHITOSAN HYDROGELS FOR DYE REMOVAL

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Urea-modified chitosan hydrogel beads were synthesized via four different methods to evaluate their potential for Congo red removal from aqueous solutions. The materials were characterized by similar point of zero charge pH_{PZC} values (6.8–7.5), indicating comparable surface charge properties, with slightly higher values observed for samples with higher urea content. Adsorption studies revealed a strong pH dependence, with maximum dye uptake at acidic conditions due to favorable electrostatic interactions. Among the prepared samples, the material containing 3% urea exhibited the highest adsorption capacity, achieving over 94% removal at 50 mg dm^{-3}. These results demonstrate that urea-modified chitosan hydrogels are promising, low-cost adsorbents for dye removal applications.

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H-13-P

GLUTARALDEHYDE-CROSSLINKED CHITOSAN/CELLULOSE HYDROGEL BEADS FOR HEAVY METAL REMOVAL: STRUCTURAL CHARACTERIZATION AND BATCH ADSORPTION EVALUATION

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The development of sustainable adsorbents for heavy metal removal remains an important challenge in water treatment. In this study, chitosan–cellulose composite hydrogel beads were synthesized and crosslinked with glutaraldehyde to improve structural stability and adsorption performance. The beads were tested for the removal of Cu(II), Pb(II), Zn(II), and Cd(II) from aqueous solutions under batch conditions. Morphological and structural characterization was performed using field emission scanning electron microscopy (FESEM) and Fourier transform infrared spectroscopy (FTIR). FESEM showed that cellulose incorporation produced a more porous, interconnected network compared to citric acid functionalized chitosan beads, while FTIR indicated corresponding structural changes in functional group interactions. Adsorption data fitted the Langmuir model, with maximum

capacities of 11.9-56.2 mg g^{-1} depending on the metal. Overall, the hydrogel beads showed good stability and efficient performance for heavy metal removal from water.

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H-14-P

LOW-COST BIOMASS-DERIVED ACTIVATED CARBONS FOR EFFICIENT Pb^{2+} REMOVAL: INFLUENCE OF ACTIVATION STRATEGY

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The increasing presence of heavy metals in aquatic environments poses a serious threat to ecosystems and human health. In this study, low-cost adsorbents derived from sawdust biomass were prepared using three different approaches: direct carbonization (P_C), physical activation with CO_2 (P_CO_2), and chemical activation with phosphoric acid (P_H_3PO_4). The materials were thermally treated at 800 °C and characterized by scanning electron microscopy (SEM), revealing significant differences in surface morphology and porosity depending on the activation method. The adsorption performance toward Pb^{2+} ions was evaluated through batch experiments, including kinetic and equilibrium studies. The chemically activated sample (P_H_3PO_4) demonstrated superior adsorption efficiency, achieving approximately 60% removal within a few hours, while CO_2-activated carbon showed moderate performance (~15%), and non-activated carbon exhibited negligible adsorption capacity (~2%). The enhanced performance of P_H_3PO_4 is attributed to its highly developed porous structure and the presence of oxygen-containing functional groups that promote metal ion binding. These findings highlight the importance of activation strategy in designing efficient biomass-derived adsorbents and demonstrate that chemically modified sawdust represents a promising, sustainable, and cost-effective solution for heavy metal removal from wastewater.

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H-15-P

SURFACE COATING TECHNOLOGIES AND FUNCTIONAL COATINGS FOR ORTHODONTIC ARCHWIRES: A REVIEW

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Nickel–titanium and stainless steel orthodontic archwires are widely used because of their favorable mechanical properties; however, prolonged exposure to the oral environment may lead to corrosion, friction, bacterial adhesion, and metal ion release. Surface coating technologies have therefore become important for improving the biological and tribological performance of orthodontic materials. This review summarizes major coating methods used in orthodontics, including Physical Vapor Deposition, Chemical Vapor Deposition, chemical precipitation, and sol–gel techniques, together with titanium-, silver-, and zirconium-based coatings. In our study, TiN-Cu nanocoatings were fabricated on NiTi archwires using combined cathodic arc evaporation and DC magnetron sputtering. The obtained coatings showed improved corrosion resistance, reduced nickel ion release, favorable biocompatibility, and significant antibacterial activity against oral bacteria.

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H-16-P

A NOVEL SYNTHESIS OF METAL SULFIDES (Ga_2S_3 AND FeS_2)

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A new approach to the synthesis of metal sulfides is proposed, taking Ga_2S_3 and FeS_2 as examples. It is found that this method permits a substantial reduction of the process temperature and, at the same time, a decrease in product contamination. In contrast to known methods for the synthesis of metal sulfides, which are based on the oxidation of halides by sulfur, the present approach employs getter substances — namely molten sodium or potassium tetrasulfides (Na_2S_4, K_2S_4) — to remove the liberated free halogen (I_2 or Br_2). The getters selectively bind the halogen, giving the corresponding sodium or potassium halides together with elemental sulfur. The synthesis of Ga_2S_3 is carried out in a two-temperature quartz reactor: at 220 °C, GaI_3 reacts with sulfur, after which, at 500–600 °C, the getter absorbs the I_2 that is liberated. It is noteworthy that when the temperature of the sulfide zone exceeds 400 °C, the monoclinic α′-Ga_2S_3 phase is formed; below 350 °C, on the other hand, the formation of the GaSI phase is likely. For the preparation of pyrite (β-FeS_2), the oxidation of $FeBr_2$ by sulfur was employed at 700 °C and $p(S_2) = 1$ bar; as a result of the binding of bromine by the getter, well-faceted crystals of pyrite (β-FeS_2) were obtained. Thus, the method permits the preparation of pure sulfides with a low residual halogen content without recourse to special vacuum equipment.

H-17-P

FROM MONO- TO BILAYER SYSTEMS: PHYSICOCHEMICAL INSIGHTS INTO Au-PNiPAAm AND Au-PNiPAAm/PVA HYDROGEL NANOCOMPOSITES

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Bilayer hydrogel nanocomposite systems have attracted increasing attention due to their potential in advanced applications, where structure strongly affects performance. It is therefore essential to understand how bilayer architecture influences physicochemical properties. In this study, mono- and bilayer hydrogel nanocomposites were prepared using a combination of chemical synthesis of gold nanoparticles (AuNPs), physical freeze-thaw crosslinking of poly(vinyl alcohol) (PVA), and gamma irradiation-induced crosslinking of poly(*N*-isopropylacrylamide) (PNiPAAm), resulting in stable structures. UV-Vis analysis confirmed the stability of AuNPs within the polymer matrix. Physicochemical characterization revealed differences between mono- and bilayer systems, indicating the combined effect of AuNPs and layer structure. Bilayer systems exhibited stable behavior and modified transport properties, highlighting the role of structural organization in swelling and diffusion mechanisms.

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H-18-P

CHEMICAL, MORPHOLOGICAL, THERMAL, AND ELECTRICAL PROPERTIES OF A NOVEL GOLD-DECORATED GMA-BASED COMPOSITE

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In this study, a novel hybrid polymer-metal system, P-NH_2@Au, was prepared via *in situ* reduction of gold precursor ions onto an amino-modified GMA-based copolymer support. FTIR analysis confirmed the successful chemical modification and the interaction between the amino groups and gold. SEM micrographs revealed a significant morphological transformation, showing distinct, bright globular gold aggregates anchored onto the porous copolymer surface. TGA performed in the 25–900 °C range demonstrated that gold incorporation altered the thermal degradation profile of the matrix,

with a residual mass of 14 wt.% providing a quantitative measure of the gold decoration. The synergy between the amino-modified copolymer and gold aggregates significantly changes the electrical resistivity, increasing from 1.91×10^3 Ωm to 12.96×10^7 Ωm. These results suggest the potential of the P-NH_2@Au composite for advanced applications in materials science.

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H-19-P

MECHANOCHEMICAL REDUCTION OF PtO_2 TO NANOCRYSTALLINE Pt USING FORMIC ACID

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A mechanochemical approach for the reduction of platinum oxide (PtO_2) to metallic platinum using formic acid was investigated. Milling was performed at 600 rpm for 30 min in a ZrO_2 reactor using a single milling ball. X-ray diffraction analysis confirmed the conversion of PtO_2 into metallic Pt with peak broadening indicating formation of nano-sized crystallites. The results show that mechanochemical treatment of platinum oxides when combined with formic acid allows the fast and efficient reduction under mild conditions providing a simple way for the synthesis of nanocrystalline platinum.

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H-20-P

PERIODATE-MEDIATED HRP IMMOBILIZATION ON MACROPOROUS COPOLYMERS: SYNTHESIS AND STABILITY ANALYSIS

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Horseradish peroxidase (HRP) is among the most frequently utilized enzymes for immobilization. While diverse supports such as alginate, magnetic beads, and silicas are available, macroporous copolymers offer distinct advantages in terms of porosity. By employing covalent binding via the periodate method, a robust linkage is established that effectively prevents enzyme leakage. In this study, HRP was successfully immobilized onto macroporous copolymer. Increased enzyme loading was found to positively correlate with biocatalytic specific activity. The immobilized system demonstrated enhanced stability and maintained effective catalytic performance over seven operational cycles.

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H-21-P

IMPACT OF MECHANOCHEMICAL ACTIVATION ON THE METASTABLE STATES AND PHOTOCATALYTIC PERFORMANCE OF AMORPHOUS HIGH-ENTROPY ALLOY RIBBONS

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Amorphous high-entropy alloy (HEA) ribbons based on the $(FeCoNiMo)_{100-x}B_x$ system were investigated before and after mechanochemical activation (MCA). The ribbons were synthesized by melt-spinning, resulting in an amorphous metastable structure. The aim of the study was to use mechanochemical treatment to stabilize the metastable cocktail-like elemental distribution and to improve the photocatalytic performance. XRD confirmed the preservation of the amorphous structure after MCA, while Mössbauer spectroscopy revealed changes in the local atomic environment and redistribution of Fe-rich and Fe-deficient regions. The photocatalytic activity of the activated samples was evaluated toward degradation of test organic pollutants. The MCA-treated alloy demonstrated significantly improved degradation efficiency, which may be attributed to improved elemental homogeneity and redistribution of the local Fe environments induced by mechanochemical activation. The obtained results demonstrate the potential of mechanochemically activated amorphous HEAs as efficient and sustainable catalytic systems for environmental protection applications.

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H-22-P

AUTOMATED MATLAB-BASED IMAGE ANALYSIS FOR PORE STRUCTURE CHARACTERIZATION OF CLAY-BASED POROUS CERAMICS

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This study presents pore structure characterization of a sintered clay material using automated MATLAB-based image processing of optical microscopy images, validated against the first bubble-point method. The clay material, sourced from the Kolubara mining basin (Serbia), was sintered at 1300 °C. The image analysis pipeline detected 5,077 individual pores, yielding a cross-sectional porosity of 21.4% and a median pore diameter (D50) of 15.0 μm. The maximum pore diameter of 127.0 μm showed 95% agreement with the bubble-point reference value (133.5 μm). The results demonstrate that automated MATLAB-based image analysis enables rapid and quantitative pore characterization with good agreement to the reference method, showing promise for microstructural characterization of clay-based porous ceramics.

Acknowledgment
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H-23-P

SYNTHESIS AND CHARACTERIZATION OF A SMART CELLULOSE-BASED HYDROGEL

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A novel cellulose-based hydrogel has been synthesized via oxidation with different molar ratios of periodate (5, 10, 15, and 20 mol %), followed by reductive amination with tyramine. UV–VIS spectroscopy and acid–base titration confirmed the modifications of the polymers. Hydrogels were formed from all four tyramine-celluloses via a cross-linking reaction catalyzed by horseradish peroxidase and hydrogen peroxide, generated from glucose and glucose oxidase. The presence of different functional groups within the same molecule enables tyramine-cellulose to change its

properties in response to external factors and to act as a smart material, making this hydrogel a promising candidate for subsequent evaluation in targeted drug delivery.

Acknowledgment
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H-24-P

SORPTION OF REACTIVE BLUE 19 BY CARBONATE-INTERCALATED LAYERED DOUBLE HYDROXIDE: INFLUENCE OF pH AND KINETIC STUDIES

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This study investigated a novel sorbent synthesized by the coprecipitation method assisted by ultrasound for the removal of Reactive Blue 19 (RB19) dye from aqueous solutions. The impact of key parameters, including contact time, initial concentration, and pH was evaluated. The obtained results were examined by non-linear regression analysis of different reaction kinetic and multi-linear diffusion models. The results indicate that the sorption of RB19 was rapid, equilibrium attained at approximately 60 minutes. The experimental sorption capacity for RB19 was 562.96 mg g^{-1}, obtained under optimal conditions at pH 2.0 with sorbent dose of 0.5 g dm^{-3}. The kinetic data suggests that the sorption process is primarily controlled by chemisorption and diffusion mechanism.

Acknowledgment
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H-25-P

ACTIVATED CARBON DERIVED FROM *Pinus nigra* CONES: SYNTHESIS AND STRUCTURAL CHARACTERIZATION

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Activated carbon derived from *Pinus nigra* cones (PNAC) was synthesized by phosphoric acid activation followed by thermal carbonization and characterized using SEM, FTIR, XRD, and nitrogen adsorption–desorption analysis. SEM revealed heterogeneous fragmented particles, while FTIR and XRD confirmed the formation of an aromatic amorphous carbon structure. The nitrogen adsorption

isotherm corresponded to Type IV with H3 hysteresis, indicating micro-mesoporous architecture. The material exhibited a BET surface area of 678 m^2/g, micropore volume of 0.2 cm^3/g, and mesopore surface area of 308 m^2/g. The methylene blue number reached 126.67 mg/g, confirming developed porosity and notable adsorption capacity.

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H-26-P

A KINETIC STUDY OF REACTIVE ORANGE 16 REMOVAL BY A BASIC BISMUTH NITRATE SORBENT

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The aim of this study was the synthesis of basic bismuth nitrate (BBN) and its application for the removal of the textile dye Reactive Orange 16 (RO16) via sorption. The material was synthesized by electrochemical deposition on a titanium cathode from an acidic bismuth nitrate solution followed by thermal treatment. The effects of the key parameters of the sorption process, such as contact time, sorbent dose, and initial dye concentration, on the sorption efficiency were investigated. The optimal conditions for the sorption process were a contact time of 1.0 min, a sorbent dose of 500.0 mg dm^{-3} and an initial dye concentration of 300.0 mg dm^{-3}. A kinetic study of the sorption process showed that dye sorption on the BBN sorbent follows pseudo-second order kinetics.

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H-27-SL

TUNING REACTIVITY WITH IMPACT: SUSTAINABLE MECHANOCHEMICAL SYNTHESIS OF MATERIALS

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Mechanochemistry, utilizing high-energy milling, is now an integral part of solid-state chemistry and is employed by numerous research groups worldwide [1,2]. This was not always the case. The lecture will offer a brief overview of the historical milestones in the development of this field and will showcase its transformation from a comminution to a synthetic tool [3]. Its basic principles and most

commonly used equipment will be described. The benefits of mechanochemistry will be demonstrated by showing decent values of green chemistry metrics for selected examples [4,5]. A description of ongoing European initiatives in this field will also be provided [6]. Examples from our laboratory will also be mentioned, specifically the processing of eggshell waste [7], the ultra-fast synthesis of metal chalcogenides via mechanically induced self-propagating reactions [8], and the preparation of bionanocomposites containing elemental silver with antibacterial activity [9].

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H-28-SL

SUSTAINABLE ENHANCED MICROWAVE SYNTHESIS OF POLYPYRROLE AND POLYPYRROLE/CHITOSAN COMPOSITES: STRUCTURAL CHARACTERISATION AND ANTIBACTERIAL PERFORMANCE

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Polypyrrole (PPy) is a widely used conductive polymer valued for its redox activity, simple synthesis, environmental stability, and strong conductivity, which it retains even at physiological pH. Its chemical synthesis typically employs oxidants such as ammonium persulfate ($(NH_4)_2S_2O_8$) or iron(III) chloride ($FeCl_3$). For effective antibacterial activity against Gram-negative and Gram-positive bacteria, PPy or polyaniline (PANI) must be synthesized under strongly acidic conditions ($pH \leq 2$) to achieve a highly doped, positively charged state. Our group recently identified potassium iodate (KIO_3) as a promising oxidant for scalable CP PANI synthesis due to its compatibility with classical and microwave-assisted polymerization and tolerance to broader reaction conditions. However, PPy synthesis using KIO_3 has not yet been reported. Furthermore, PPy's poor solubility limits its processability, prompting interest in composites with biopolymers such as chitosan (Ch), which offers biocompatibility and structural support.

Microwave (MW) irradiation provides a rapid, energy-efficient route for polymer nanomaterial synthesis. Conventional MW heating rapidly raises the reaction temperature but delivers energy only during active irradiation, limiting its use for CP synthesis. Our group recently developed an enhanced MW method that maintains constant temperature while continuously delivering MW energy, enabling ultrafast CP PANI synthesis within minutes and offering fine control over morphology in comparison to classical chemical synthesis (CS) method.

In this study, PPy and PPy/Ch composites were prepared for the first time using a sustainable, rapid, and convenient enhanced-microwave method conducted at ambient temperature, employing oxidising agents such as standard oxidising agent $(NH_4)_2S_2O_8$ and KIO_3 oxidising agent to support industrial scalability. Physical and morphological properties of the PPy, and PPy/Ch synthesised using medium-molecular-weight Ch were investigated. A comparative assessment of PPy and PPy/Ch samples produced by either CS or enhanced microwave (MW) method and using either $(NH_4)_2S_2O_8$ or KIO_3 oxidising agent was conducted with respect to their structural, morphological and antibacterial properties. Understanding the factors which affect the formation of PANI nanofibers in the composite using enhanced MW approach, together with the findings based on CS approach can help tuning PPy formation conditions toward the particular properties of PPy composites for various applications.

H-29-SL

THERMAL DECOMPOSITION OF TITANIUM AMMONIUM FLUORIDE

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Ammonium titanium fluoride is one of the important intermediate products in the research strategy of red mud treatment. After red mud reduction using hydrogen or carbon, the separated solid residue was dissolved in concentrated acid and the resulting pregnant solution was subjected to solvent extraction in order to selectively separate titanium from iron, aluminum and other elements. The obtained solution of ammonium titanium fluoride was treated by ultrasonic spray pyrolysis method in a neutral atmosphere forming spherical particles of titanium oxide. The thermal decomposition of ammonium titanium fluoride was analyzed using thermogravimetric and differential thermal analysis. Scanning electron microscopy, energy dispersive X-ray spectroscopy EDX and X-ray structural analysis were used to analyze the composition, structure and morphology of particles. The influence of temperature on particle size was investigated between 500°C and 1000°.

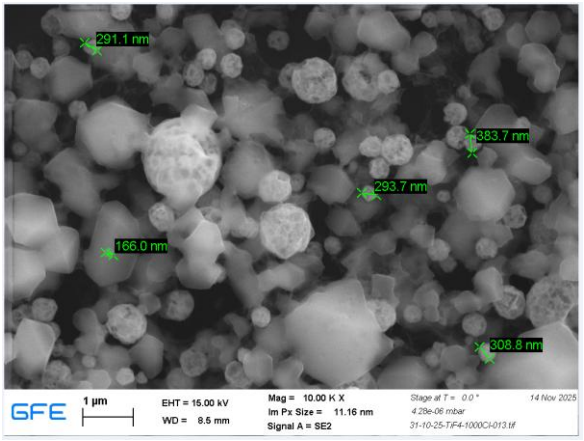

Figure 1. The particles obtained by thermal decomposition of ammonium titanium fluoride via ultrasonic spray pyrolysis in neutral atmosphere

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J *– Macromolecular Physical Chemistry*

J-01-P

THE INFLUENCE OF COLOR ADITIVES ON THE STRUCTURE AND THERMAL PROPERTIES OF POLY(LACTIC ACID)

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In terms of the potential application as 3D printing materials, poly(lactic acid) (PLA), commercially available and known as Wanhao PLA Filament, was investigated. The impact of incorporated color additives on the structure and thermal properties of the PLA was examined. The obtained results show that the incorporation of different colors has no impact on the structure, while on the other hand it has noticeable impact on the thermal stability of the examined PLAs.

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J-02-P

THE SYNTHESIS AND STRUCTURE OF THE WATERBORNE POLYURETHANE-UREAS BASED ON POLYCAPROLACTONE

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A series of waterborne polyurethane-ureas (WBPUUs), based on polycaprolactone (PCL), isophorone diisocyanate (IPDI), 2,2-bis-(hydroxymethyl) propionic acid (DMPA), triethylamine (TEA) and ethylene diamine (EDA) as a chain extender, was successfully synthesized. Different –NCO/–OH molar ratios (1.3, 1.4 and 1.5) have been applied in order to prepare three WBPUU films. The structure of so prepared WBPUUs has been examined in detail by FTIR and NMR spectroscopy.

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J-03-P

RHEOLOGICAL PROPERTIES OF HYPERBRANCHED POLYESTERS

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Two hyperbranched polyesters (HBPs) of the fourth pseudo generation were synthesized from dimethylolpropionic acid (DMPA) as AB_2-type monomer and di-trimethylolpropane (DiTMP) as B_4 functional core. Both samples were prepared in an acid-catalyzed polyesterification reaction in melt, using pseudo-one-step (HBP1) or one-step (HBP2) procedure. Pseudo-one-step procedure implicates utilization of previous pseudo generation HBP and stoichiometric amount of DMPA to prepare the next pseudo generation HBP, while during one-step procedure adequate amount of DMPA is added to the DiTMP core at once. Rheological properties of the synthesized HBPs were compared between each other, as well as with properties of the commercial HBP of the fourth pseudo generation, synthesized via pseudo-one-step procedure from DMPA and tetrafunctional ethoxylated pentaerythrytol (PP50) core.

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J-04-P

ENERGETICS OF POLYMER NANO-PARTYICLES UPTAKE BY CELLS: I. The scaling theory approach to transport phenomena at living cell level

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The energy needed for uptake of typical polymer nano particles into living cells is analyzed for a set of systems with poly lactic acid and its copolymers, and different cell types, using Helfrich Hamiltonian and set of models, later developed from it, but considering in addition the impact of cell ATP level, what is approach applied for the first time. The results point to the endocytosis mechanism complexity, the impact and importance of the new area of macromolecular physical chemistry, for understanding those phenomena at nano level to be illustrated in 3 papers (noted Part I, II, and III) at this Conference, with the same main title.

J-05-P

ENERGETICS OF POLYMER NANO-PARTICLES UPTAKE BY CELLS: II. The kinetics of cells uptake of drugs, in some aspects of membrane liquid crystalline states theory

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Some trends of general characters are presented, from the revisiting our earlier experimental data and a large pull of published data on similar systems on targeted drug release kinetics by cell responding to drug deriver. The described cell behavior by nano particles uptake is related to modern theories on cell membrane structure, very similar to polymer liquid crystals and the new ideas on needs to include phospholipids into macromolecular class of structures, despite their low molar mass. The issues are of a fundamental importance also because same mechanisms are active by RNA vaccines and gene vector endocytosis, but also by some viruses enter into the cells.

J-06-P

ENERGETICS OF POLYMER NANO-PARTICLES UPTAKE BY CELLS: III. Some thermodynamic aspects of cell uptake mechanisms

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The unique physicochemical states, created by self-suspending polymer nano-particles, what are different principles than in macro suspensions and emulsions, are considered in theoretical and experimental approach, especially for better understanding some receptor mediated cell uptake. It can be also of high importance for pharmacokinetics, medicine and high technologies by design of nano-enhanced phase change materials, for thermal energy storage and its transfer in electronics.

K *– Environmental Protection,*
Forensic Sciences,
Geophysical Chemistry,
Radiochemistry,
Nuclear Chemistry

K-01-P

ACTIVATED FLAX FIBERS/FLY ASH ADSORBENTS FOR HEAVY METAL REMOVAL FROM WATER

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The hybrid adsorbents were synthesized by thermal treatment and activation of waste flax fibers and fly ash, and used for the adsorption of zinc and cadmium ions. The adsorption performance was systematically evaluated by examining the influence of initial solution pH, metal ion concentration, contact time, and temperature. The results indicate that the adsorbent with a higher proportion of flax fibers exhibits superior adsorption performance, achieving Langmuir maximum adsorption capacities of 66.7 mg g^{-1} for Zn(II) and 9.02 mg g^{-1} for Cd(II). The adsorption process is best described by the pseudo-second-order kinetic model and the Langmuir isotherm, suggesting monolayer adsorption on a relatively homogeneous surface. Furthermore, thermodynamic analysis supports a chemisorption-dominated mechanism. These results highlight the potential of such hybrid materials as sustainable and cost-effective adsorbents.

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K-02-P

SURFACE-MODIFIED DIATOMACEOUS EARTH AS A LOW-COST ADSORBENT FOR CATIONIC DYE REMOVAL

Marina Maletić [1], Marija Vukčević [2], Irina Miletić [2], Danica Janković [2], Aleksandra Perić Grujić [2], and Katarina Trivunac [2]

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This study compares two adsorbents based on diatomaceous earth modified with magnesium and barium carbonate for the removal of methylene blue and brilliant green from aqueous solutions. The modified materials were characterized, and their adsorption performance was assessed by examining the effects of pH, contact time, and initial dye concentration. FTIR spectra confirmed successful carbonate modification of diatomaceous earth, and SEM analysis revealed differences in surface porosity and heterogeneity between barium and magnesium carbonate-modified materials. The

results indicate rapid adsorption for both dyes, with a better fit to the pseudo-second-order kinetic model. Adsorption efficiencies increase with the pH of the dye solution, reaching especially high Langmuir adsorption capacities of 322.6 and 298.5 mg/g for the adsorption of brilliant green on barium and magnesium carbonate-modified materials, respectively. The barium carbonate-modified material exhibited higher adsorption capacities for both dyes, confirming the potential of modified diatomaceous earth as an effective, low-cost adsorbent for dye removal.

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K-03-P

INVESTIGATION OF GEOCHEMICAL SULFATE INTERACTIONS WITH NATURE-BASED SILICATE GEOMATERIALS IN SURFACE WATERS: LEACHING VERSUS SORPTION

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This study investigates sulfate (SO_4^{2-}) interactions of five nature-based silicate geomaterials (NBSG) - pyrophyllite schist, perlite, vermiculite alterite, zeolitic tuff, and sand - in water matrices from the Bor (Serbia) mining region (Kriveljska River and Green Lake). Results show that for pulverized NBSG, geochemical interaction is dominated by leaching rather than sorption. While sand achieved marginal removal (<20%) in river water, no removal occurred in the lake. Conversely, other NBSG induced a substantial SO_4^{2-} increase due to mineral leaching. To assess total geochemical impact, a Net Interaction Balance (NIB) was calculated, including primary leaching and citric acid-triggered mobilization. Findings reveal significant SO_4^{2-} release potential, with NIB values reaching +822.66 mg/L for sand in the lake matrix. This study establishes a baseline, emphasizing that NBSG application must be preceded by rigorous validation to prevent inadvertent water quality degradation.

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K-04-P

MONITORING THE EFFECTS OF PFAS CHEMICALS ON PHOTOSYNTHESIS AND CELLULAR RESPIRATION OF WHEAT (*Triticum aestivum L.*) USING THE COLUMBUS MICRO-OXYMAX RESPIROMETER

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Per- and polyfluoroalkyl substances (PFAS) are a group of persistent organic pollutants widely distributed in the environment due to intensive industrial use and notable chemical stability. Among the most significant representatives are perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS). Phytoremediation is considered a viable approach to remove PFAS chemicals from contaminated environments, but knowledge of the physiological responses of plants to these compounds remains limited. Therefore, the aim of this study was to investigate the influence of PFOA and PFOS on cellular respiration and photosynthetic activity in wheat (*Triticum aestivum L.*) using the Micro-Oxymax respirometer. Wheat seeds were grown in nutrient media supplemented with PFOA and PFOS at concentrations of 1 and 10 ppm. Over 13 days, cumulative production of oxygen and carbon dioxide was monitored. The control group showed the highest cumulative production of O_2 (511.78 mL) and CO_2 (31.47 mL), while all PFAS treatments resulted in decreased plant metabolic activity. A more pronounced inhibitory effect was observed with the application of 10 ppm PFOA and both concentrations of PFOS, where O_2 production was approximately half that of the control. The results indicate that PFAS compounds negatively affect the physiological processes of wheat.

Acknowledgment
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K-05-P

A COMPARATIVE BIOSORPTION OF TOLUIDINE BLUE WITH AMBROSIA-BASED BIOSORBENTS

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The major sources of water pollution in the environment are industrial activities whose wastewater often contains contaminants, such as synthetic organic dyes. These compounds can be toxic to living organisms, including humans, and their removal from wastewater is essential. Biosorption as a technique that uses materials of biological origin, is considered simple, inexpensive, and environmentally friendly. In this study, the biomass of *Ambrosia artemisiifolia* was used as a biosorbent for the removal of synthetic organic dye Toluidine Blue (TB). Experiments were conducted using non-magnetic (NMB), and magnetic (MB) Ambrosia-based biosorbents. The removal efficiency of the biosorbents was evaluated using UV-Vis spectroscopy. Additionally, the biosorbents were characterized before and after biosorption process, using Attenuated total reflection Fourier transformed infrared spectroscopy (ATR-FTIR). After 2 hours of biosorption process, the removal efficiency of TB was 99% for NMB, and 100% for MB.

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K-06-P

NON-LINEAR REGRESSION ANALYSIS OF SELENIUM SORPTION ONTO AMINO-MODIFIED GMA-BASED NANOCOMPOSITE: KINETIC AND EQUILIBRIUM STUDY

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In this paper, selenium sorption from aqueous solutions was investigated using a porous glycidyl methacrylate (GMA)-based nanocomposite modified with diethylenetriamine at pH 6.0. The effects of contact time, initial selenium concentration, and temperature on selenium sorption were evaluated, and kinetic and equilibrium parameters were determined using non-linear regression analysis. The kinetic data are best described by the Avrami kinetic model, indicating a complex sorption mechanism. The results of non-linear fitting show that the Langmuir model most adequately describes the equilibrium data, with a maximum sorption capacity of 1.26 mg/g. The mean free energy of sorption calculated from the Dubinin-Radushkevich model (E = 15.07 kJ/mol) confirms that the dominant mechanism of selenium removal is ion exchange.

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K-07-P

DEPTH DISTRIBUTION OF SOIL PROPERTIES IN SILTY LOAM SOIL IN RELATION TO LONG-TERM WATER EROSION ASSESSED BY ^{137}Cs

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Although water erosion is a global threat to soil resources, its effects on the vertical stratification of soil properties remain insufficiently quantified. This study examines the relationship between long-term erosion rates, derived from ^{137}Cs measurements, and the depth distribution of physical and chemical properties in erosion-prone silty loam soils. While soil pH and electrical conductivity (EC) were highest at the surface (0–5 cm), soil texture exhibited depth-dependent patterns, with clay content increasing and coarse fractions decreasing toward the 20–25 cm depth. Erosion rates correlated significantly with textural differentiation ($\Delta_{\text{0-5 vs 20-25 cm}}$), whereas no relationships were observed for pH or EC. Results indicate that long-term erosion is associated with vertical differentiation of soil texture, leading to surface coarsening. These structural modifications increase the contrast between soil layers, potentially reducing water retention and accelerating soil degradation.

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K-08-P

EVALUATION OF HEALTH RISKS ASSOCIATED WITH HEAVY METALS IN SURFACE WATER OF THE OBRENOVAC AREA

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Heavy metal contamination of river water may pose potential risks to human health, especially near urban and industrial areas. In this study, water samples were collected from the Kolubara River and its tributaries near Obrenovac, Serbia, and concentrations of Pb, Zn, Cu, Mn, Cd, Ni, Fe, Hg, Co, and Cr were determined. Non-carcinogenic and carcinogenic health risks for adults and children were

assessed through ingestion and dermal exposure pathways. The obtained non-carcinogenic risk ranged from 0.04 to 1.02 for adults and from 0.10 to 2.47 for children, while carcinogenic risk ranged from 1.59×10^{-5} to 3.56×10^{-4} and from 7.97×10^{-6} to 1.78×10^{-4}, respectively. Chromium was the dominant contributor to both risk types. Although most samples indicated acceptable risk levels, certain locations downstream of Obrenovac suggest possible local contamination and highlight the need for continuous monitoring.

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K-09-P

MULTIVARIATE ANALYSIS OF RIVER SEDIMENT IN THE VICINITY OF NOVI PAZAR, SERBIA

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Sediments provide both habitat and a nutrient source for aquatic organisms, which is why sediment pollution levels are of great importance to overall environmental quality. In this study, river sediment from the vicinity of the city of Novi Pazar, Serbia, was analyzed in order to determine heavy metal (HM) concentrations and identify their potential sources. A total of nine HMs were analyzed, including Cd, Sb, Fe, Cr, Cu, Mn, Ni, Pb, Zn. The Pearson correlation matrix, hierarchical cluster analysis (HCA), and principal component analysis (PCA) were applied to investigate the complex relationships among HMs and to assess their potential sources. Based on the applied multivariate analysis, it was determined that anthropogenic activities are the dominant contributors to elevated HM concentrations in the sediments. In addition, certain HMs, such as Cr and Ni, were found to originate from both anthropogenic and natural sources.

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K-10-P

DIURNAL AND SEASONAL DYNAMICS OF AMBIENT GAMMA DOSE RATE AND ITS RELATIONSHIP WITH METEOROLOGICAL PARAMETERS AND PARTICULATE MATTER IN KRUŠEVAC, SERBIA

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Natural background radiation is largely influenced by meteorological and atmospheric dynamics. In radiation monitoring networks, this may pose a challenge when distinguishing changes attributable to radiological events from routine fluctuations. This study examines diurnal and seasonal patterns of the ambient gamma dose equivalent rate, $\dot{H}^*(10)$, measured in 2024 at a radiation monitoring station in Kruševac, Serbia, and its relationships with selected meteorological variables and particulate matter. The results indicate significant differences in $\dot{H}^*(10)$ values between seasons and between daytime and night-time periods. The most pronounced diurnal cycles were observed during summer and autumn and are attributed to dynamics of the atmospheric boundary layer. Correlation analysis identified temperature, relative humidity, and precipitation as the main meteorological modulating factors, while particulate matter was found to act as a carrier of radon progeny, particularly in autumn.

K-11-P

RADIOLOGICAL HAZARD IN SOILS AFFECTED BY NORM RESIDUES FROM THE PHOSPHATE INDUSTRY: PRAHOVO, SERBIA

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This study presents an assessment of the radiological hazard of topsoil in the vicinity of a major phosphate industrial facility in Prahovo, eastern Serbia. Fifty-five topsoil samples were analyzed by HPGe gamma-spectrometry for the activity concentrations of ^{226}Ra, ^{232}Th, and ^{40}K, and the results were used to determine the absorbed dose rate, annual effective dose, excess lifetime cancer risk, and external hazard index. Additionally, the ambient dose equivalent rate was measured *in situ* at each sampling location and spatially modeled using ordinary kriging to delineate the radiological footprint of the study area. The absorbed dose rate (mean 52 nGy h^{-1}) was comparable to the national average, and the hazard index remained below unity at all sampling locations, while spatial analysis revealed localized elevations of the ambient dose equivalent rate near the river port and legacy phosphogypsum deposits within the industrial zone.

K-12-P

A LAB SCALE STUDY ON ORGANIC LOADING REMOVAL FROM REAL MUNICIPAL WASTEWATER USING AN SOLAR PHOTOCATALYTIC MEMBRANE REACTOR

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This study demonstrates the functionality of an experimental solar Photocatalytic Membrane Reactor (PMR) designed for the removal of organic load (measured as Chemical Oxygen Demand - COD) from real municipal wastewater. The research focused on evaluating the performance of a 1% wt. Fe-TiO_2 photocatalyst (prepared via well-known sol-gel method) under simulated solar light. All experiments achieved total COD removal efficiencies exceeding 80%. Final COD concentrations in treated samples were reduced to between 8.8 and 26.4 mg O_2/L, well within safe environmental discharge standards. These results confirm that the solar PMR model, combining photocatalysis using iron-doped titanium dioxide and polymeric membrane separation, is a highly effective and sustainable solution for advanced wastewater treatment.

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K-13-P

STUDY ON MUNICIPAL MIXED SOLID WASTE TRANSFORMATION TO REFUSE DERIVED FUEL AS AN ALTERNATIVE FOR ENERGY PRODUCTION

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This study investigates the production of refuse-derived fuel (RDF) from municipal solid waste fractions, including mechanically treated waste, composting reject material, municipal sewage sludge, and potato starch as a binder. Raw materials were physically and chemically characterized through elemental analysis, heavy metal quantification via ICP-MS, and gross calorific value measurement. Three fuel blends were formulated and benchmarked against commercial charcoal briquette standards for moisture, ash, chlorine, sulphur, and heating value. All mixtures demonstrated calorific values between 22.0 and 23.1 MJ/kg, well above the minimum incineration threshold of 7 MJ/kg and close to commercial charcoal at 25 MJ/kg. Chlorine and Sulphur contents remained within acceptable limits. Although density decreased after 24 hours, all mixtures-maintained stability over 30 days. These findings confirm that waste-derived fuel blends represent viable alternative fuels with combustion properties approaching commercial charcoal, supporting sustainable municipal waste valorization.

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K-14-SL

AI-AGENTIC SYSTEM FOR AUTOMATED STATISTICAL PROCESSING OF AGRICULTURAL DATA WITH A LOCALLY DEPLOYED LLM AND DOMAIN-SPECIFIC STATISTICAL ONTOLOGY

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Reliable statistical analysis of agricultural and agrochemical data is a critical prerequisite for drawing valid scientific conclusions and for supporting risk-sensitive decisions in crop production and land management. However, many domain experts still rely on ad-hoc analytical workflows and suboptimal statistical choices, which limits reproducibility and slows down research. In this work, we propose an agent-based framework that automates key steps of statistical data analysis for agro-environmental studies by combining a locally deployed LLM with a semantic layer for statistics.

The core idea is to represent methodological knowledge as a domain-specific ontology and a methodological graph that encode: (i) typical data structures and variable types in agrochemical and field-experiment datasets, (ii) assumptions about distributions, dependence and sampling schemes, and (iii) decision rules for selecting appropriate statistical tests, models and diagnostic procedures. On top of this semantic layer we implement a set of cooperative AI-agents. A "statistical reasoning" agent interprets the user's scientific question, inspects the dataset, traverses the methodological graph and validates the used analytical pipelines and suggests improvements. A "tool-calling" agent executes these pipelines using open-source statistical packages (R, Python), while a "validation" agent checks assumptions and reports diagnostic metrics in a transparent, reproducible format.

The use of a local LLM ensures data locality and controllability, while the semantic constraints mitigate hallucinations and enforce statistically sound choices. We illustrate the approach on agrochemical monitoring datasets and multi-factor field trials, showing how the system reduces analysis time, improves consistency of methodological decisions and can be extended to other agricultural domains.

L *– Phase Boundaries,*
Colloids,
Liquid Crystals,
Surface-Active Substances

L-01-P

ENHANCEMENT OF ALKALINE DEGREASING PERFORMANCE BY ADDITION OF LAURYLAMINE OXIDE AND NONIONIC SURFACTANT

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Alkaline degreasers are widely used in industrial cleaning but often suffer from limited wetting, emulsification, and soil redeposition issues. This study evaluates the enhancement of degreasing performance by incorporating laurylamine oxide (LAO) in combination with a nonionic surfactant (alcohol ethoxylate). Model formulations were prepared and tested for oil removal efficiency, surface tension, emulsification stability, and redeposition behavior. The results show a strong synergistic effect, with up to 35% improvement in oil removal efficiency compared to the base formulation. The addition of LAO significantly reduces surface tension, improves emulsion stability, and minimizes redeposition. Optimal performance was achieved at 0.5 – 1.0% LAO. Obtained results demonstrate that LAO is an effective co-surfactant for enhancing alkaline degreasing systems in industrial applications.

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M – Complex Compounds

M-01-P

PREPARATION OF NEW MIXED LIGAND Lu(III) COMPLEX

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Radionuclides and radiopharmaceuticals are widely used in medicine as diagnostic markers or as irradiators in therapy. Their application is constantly evolving and has become very important for clinical practice. This is precisely why there is growing interest in the synthesis of new lanthanide complexes with macrocyclic ligands.

This paper reports the synthesis of a novel mixed ligand Lu (III) complex with tpmc = N,N', N'',N'''-tetrakis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane and two additional chloro and aqua ligands. Composition of isolated complex proposed by: elemental analysis (C, H, N) and FTIR spectra. The analytical data show the formation of binuclear $[Lu_2tpmcCl_2(H_2O)_2](BF_4)_4 \cdot 2NaBF_4$ complex.

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M-02-P

DFT AND MOLECULAR DOCKING STUDY OF THE INTERACTION OF Mo, Ru, AND Os PHENANTHROLINE COMPLEXES WITH DNA

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The interaction of Mo, Os, and Ru phenanthroline complexes with DNA was investigated using DFT, EDA, and DOCKER calculations. DOCKER was used to generate possible minor groove binding poses and compare relative interaction energies. Selected structures were further analyzed by DFT interaction energy calculations and EDA. The DOCKER results suggested comparable binding strengths for Os and Ru, while DFT calculations showed similar interaction energies for the selected Mo and Os structures and a lower interaction energy for the Ru structure. EDA confirmed that dispersion and electrostatic interactions are the dominant attractive contributions, while Pauli repulsion opposes binding. These results show that the studied metal complexes form stable noncovalent interactions with DNA, mainly governed by dispersion and electrostatic effects.

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M-03-P

CH/O HYDROGEN BONDS OF 1,10-PHENANTHROLINE AND ITS TRANSITION METAL COMPLEXES: QTAIM ANALYSIS

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CH/O interactions between water molecule and the free and coordinated 1,10-phenanthroline (phen) molecule are analyzed by Quantum Theory of Atoms in Molecules (QTAIM). The results confirm the presence of interactions of non-covalent type, while the covalent character is practically not present in these interactions. QTAIM parameters do not correlate well enough to total interaction energies to be used as reliable descriptors for CH/O total interaction energy.

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M-04-P

QTAIM ANALYSIS OF INTERACTIONS IN HYDROQUINONE DIMER

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Intermolecular interactions of hydroquinone are of great importance because of their relevance in various fields. In this work, we retrieved seven crystal structures of hydroquinone dimers bonding via different non-covalent interactions. The chosen structures represent two types of hydrogen bonds, a CH···π interaction, two π-π stacking interactions on small offsets, and two on large offsets. We performed Quantum Theory of Atoms In Molecules (QTAIM) analysis to obtain further insights into these non-covalent interactions, and combined these findings with previously calculated interaction energies between hydroquinones. We have shown that QTAIM analysis is very useful to find additional, weaker interactions through the existence of their bond critical points (BCP). However, we didn't find correlation between QTAIM parameters and total interaction energies, which suggests

that QTAIM parameters corresponding to the BCPs are not a good predictor of the interaction energy strength.

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M-05-P

THE STRENGTH OF EXPERIMENTAL CH/O HYDROGEN BONDS OF COORDINATED 1,10-PHENANTHROLINE WITH WATER

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Weak CH/O interactions of 1,10-phenanthroline (phen) can become almost as strong as water-water hydrogen bonds when phen is coordinated. Model systems with linear CH/O hydrogen bonds exhibit interaction strengths up to −4.42 kcal/mol, which is a substantial increase compared with the strongest interaction of uncoordinated phen, −2.57 kcal/mol. To broaden our understanding of CH/O interactions of coordinated phen, we calculated interaction energies for various types of CH/O hydrogen bonds found in crystal structures, thereby expanding this investigation to experimental geometries. We selected six crystal structures with different CH/O types and complex charges but similar hydrogen bond lengths and calculated interaction energies at B3LYP-D4/def2-TZVP level. The resulting interaction energies range from a very weak −0.73 kcal/mol for neutral complex to very strong CH/O interactions for +2 charged complexes, reaching −6.38 kcal/mol, which indicates their significance for crystal packing.

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N – General Physical Chemistry

N-01-P

ELECTROCHEMICAL DEGRADATION OF IBUPROFEN USING SnO_2-MWCNT@SS ANODE: KINETICS OF A DECAYING RATE CONSTANT

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The electrochemical degradation of ibuprofen (IBP), a persistent pharmaceutical pollutant, was investigated using a nanostructured tin dioxide–multiwall carbon nanotube anode (SnO_2-MWCNT@SS). A first-order kinetic model with an exponentially decaying rate constant was applied to interpret the degradation profile. The model provided an excellent fit to the experimental data (R^2 = 0.9984), yielding an initial rate constant k_0 of 0.89 h^{-1} and a decay constant α of 1.21 h^{-1}. The short half-life of the rate constant (0.6 hours) indicates a rapid loss in the system's oxidative capacity over time. These findings suggest that electrooxidation targets IBP sites with heterogeneous reactivity, where readily oxidizable positions are consumed first, leaving more recalcitrant structures. This insight highlights a fundamental kinetic limitation and directs future strategies toward maintaining catalytic efficacy for complete pollutant mineralization.

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N-02-P

WASTE TO FUNCTION: ELECTROCHEMICAL PERFORMANCE OF THERMALLY CONVERTED PHARMACEUTICAL RESIDUES

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The increasing generation of pharmaceutical waste represents an environmental challenge with potential for its conversion into functional electroactive materials. In this study, expired pharmaceutical products were thermally treated at 800 °C to obtain inorganic residues used as electrode-modifying material. The obtained powder was characterized by scanning electron microscopy (SEM) and X-ray powder diffraction (XRPD), revealing heterogeneous oxide phases with irregular morphology. The calcined material was deposited onto an electrode surface and investigated electrochemically as a model system. The electrochemically active surface area (ECSA)

was determined at different mass loadings. Results show that ECSA increases with increasing mass, but deviates from linearity at higher loadings due to reduced accessibility of active sites and partial pore blocking. These findings indicate that thermally treated pharmaceutical residues exhibit measurable electrochemical activity, strongly dependent on surface accessibility and deposition amount. The study demonstrates a simple route for transforming pharmaceutical waste into low-cost electroactive materials with potential application in electrochemical systems.

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N-03-P

DETERMINATION OF NAPROXEN IN WASTEWATER BY GC–MS USING TRIMETHYLSILYL DERIVATIVES

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Pharmaceutical residues, particularly non-steroidal anti-inflammatory drugs (NSAIDs), are increasingly detected in aquatic environments due to their extensive use and incomplete removal in wastewater treatment plants. This study aimed to develop and validate a GC–MS method for naproxen determination in wastewater after derivatization to its trimethylsilyl ester form and to evaluate extraction efficiency using different solvents. Efficient chromatographic separation was achieved on a nonpolar stationary phase, while characteristic fragment ions (m/z 185, 243, 287, and 302) enabled reliable identification and quantification. Both solvents showed satisfactory reproducibility RSD (≤ 3.0%), but dichloromethane provided higher recovery (96.0%) compared to diethyl ether (77.3%). The developed method proved reliable, precise, and suitable for naproxen analysis in wastewater samples.

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N-04-P

INFLUENCE OF STORAGE CONDITIONS ON THE FLUORESCENCE RESPONSE OF WALNUT (*Juglans regia* L.) POLLEN

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The fluorescence behavior of walnut (*Juglans regia* L.) pollen stored under different environmental conditions was investigated. Pollen samples were kept under room-temperature, frozen, humid, and dry conditions. Fluorescence emission spectra were recorded under UV excitation to evaluate storage-induced changes. Distinct differences in fluorescence spectral profiles were observed among the storage treatments. Frozen pollen exhibited the smallest changes in emission band position and overall spectral shape relative to fresh pollen, whereas humid and dry storage conditions induced more pronounced spectral modifications. Dry-stored pollen exhibited better fluorescence preservation compared with room-temperature storage. The results confirm that environmental conditions strongly affect the fluorescence properties of walnut pollen and demonstrate the potential of fluorescence spectroscopy as a rapid and non-destructive method for monitoring pollen preservation and storage stability.

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N-05-P

LASER DESORPTION/IONIZATION MASS SPECTROMETRY FOR THE ANALYSIS OF OLEIC ACID-FUNCTIONALIZED $CoFe_2O_4$ NANOPARTICLES

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Laser desorption/ionization mass spectrometry (LDI-MS) enables direct characterization of oleic acid-coated $CoFe_2O_4$ nanoparticles without prior sample preparation or the use of an external matrix. Positive ion mode analysis provides evidence for the chemical binding of oleic acid to surface metal centers. In particular, the ion observed at *m/z* 685 can be identified as $CoFe_2O_3(OH)(C_{18}H_{33}O_2)_2 - CH_3(CH_2)_7$ or $CoFe_2O_4(C_{18}H_{34}O_2)(C_{10}H_{17}O_2)$, along with their corresponding fragment ions (at *m/z* <685). In negative ion mode, the LDI mass spectrum confirms the presence of oleic acid on the cobalt ferrite surface by detecting the deprotonated molecular ion at *m/z* ~281 and its characteristic fragment ions. The LDI-MS results are consistent with previous FTIR results. Overall, LDI–MS is a powerful tool for detecting inorganic–organic cluster formation and provides valuable insight into the role of surfactants in nanoparticle stability and dispersion, which is an important aspect of their application.

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O *– Pharmaceutical Physical Chemistry*

O-01-P

ELECTRONIC PROPERTIES AND REACTIVITY OF GEFITINIB, AKG2 AND SirReal2: A DFT APPROACH

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DFT analysis of AKG2, gefitinib, and SirReal2 at the B3LYP/6-31G(d,p) level was performed to evaluate their electronic properties relevant for potential tyrosine kinase/SIRT dual inhibition. The values of quantum-chemical descriptors, distributions of molecular orbital and molecular electrostatic potential suggest that all three compounds possess both electron donor and electron acceptor characteristics. These findings provide a basis for further experimental investigation of redox properties and support the design of novel dual-target inhibitors.

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O-02-P

DFT INSIGHT INTO THE ELECTRONIC PROPERTIES OF THIOSEMICARBAZONE-BASED COMPOUNDS

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A series of 28 thiosemicarbazone-based compounds was investigated at the B3LYP/6-31G(d,p) level to evaluate their electronic properties and potential structure–activity relationships. The distribution of frontier molecular orbitals, electrostatic potential maps, as well as values of MEP_{min}, MEP_{max}, E_{HOMO}, E_{LUMO} and quantum chemical reactivity descriptors indicate that most compounds exhibit similar electronic profiles. Subtle differences in charge distribution and the overall electronic environment may influence their metal ion chelation properties.

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O-03-P

IN SILICO MODELLING OF HDAC3 AND HDAC6 INHIBITORS

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Several *in silico* methodologies, including machine learning (ML), molecular docking, and quantum chemical simulations, were employed to identify structural features governing inhibitory activity toward two histone deacetylase (HDAC) isoforms, HDAC3 and HDAC6. The ML models exhibited high performance, with accuracy, recall, precision, and F1-score values close to unity for HDAC3 and approximately 0.98 for HDAC6, demonstrating strong robustness and generalizability. Furthermore, the combined application of these methodologies provided insight into how substituent reactivity and size influence inhibitory potency across the binding site.

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O-04-P

MACHINE LEARNING–BASED MODELING OF SELECTIVE CLASS IIA HDAC INHIBITORS

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This study aims to develop a machine learning (ML) model for predicting the selectivity of class IIa histone deacetylase inhibitors, which are key enzymes involved in epigenetic regulation and cancer-associated gene expression. To address the challenges posed by small and class-imbalanced datasets, we adopted a strategy based on coupling binary classification models for each isoform. For all four isoforms, five ML algorithms were evaluated in combination with MACCS keys as molecular features. Among them, the Random Forest algorithm achieved the best performance, with Matthews correlation coefficient values exceeding 0.79 and balanced accuracy, recall, precision, F1-score, and area under the receiver operating characteristic curve all exceeding 0.94. Comparable external validation metrics were also obtained for models predicting inhibitor selectivity across isoforms, confirming the robustness and generalizability of the proposed approach.
Acknowledgment

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O-05-P

NEUROADAPTIVE CHANGES IN THE RAT PREFRONTAL CORTEX FOLLOWING ZALEPLON WITHDRAWAL: BEHAVIORAL AND MOLECULAR EVIDENCE

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Zaleplon is a hypnotic with high selectivity for the alpha subunit of the gamma-aminobutyric acid (GABA) type A receptor (αGABA$_A$R). Although introduced as safe alternative to the habit-forming benzodiazepines, our study examined the effects of zaleplon withdrawal after 5-day treatment on anxiety-like behavior and the GABAergic system in the rat prefrontal cortex. Open Field Test was performed 24h after the last dose to assess the withdrawal phase, and protein expression of glutamic acid decarboxylase (GAD65/67), vesicular GABA transporter (VGAT), and the αGABA$_A$R was analyzed using Western blot. Zaleplon-treated rats showed increased anxiety-like behavior. Downregulation of α subunit of gamma-aminobutyric acid (GABA)$_A$ receptor likely mediates the observed rebound anxiety, while increased GAD65/67 and VGAT suggests a failed compensatory response to restore inhibitory tone. These findings highlight the GABAergic dysregulation even after short-term exposure to selective hypnotic agents.

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O-06-P

NEUROSYNAPTIC REMODELLING IN THE AMYGDALA DURING BENZODIAZEPINE WITHDRAWAL: EVIDENCE FROM AN ALPRAZOLAM DISCONTINUATION MODEL IN FEMALE WISTAR RATS

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Benzodiazepine withdrawal is associated with anxiety, neuronal hyperexcitability, and altered emotional processing, but the underlying synaptic mechanisms remain insufficiently understood. This

study examined neurosynaptic remodeling in the amygdala during alprazolam withdrawal in female Wistar rats. Animals received escalating doses of alprazolam for eight days, followed by abrupt discontinuation. Synaptic protein expression was analyzed by Western blot, and extracellular glutamate levels were measured using a colorimetric assay. Withdrawal produced significant neuroadaptive changes in synaptic proteins of both inhibitory and excitatory neurotransmission, along with increased extracellular glutamate levels. These results indicate a disrupted excitatory–inhibitory balance and marked synaptic remodeling in the amygdala during alprazolam withdrawal.

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O-07-P

REGION-SPECIFIC DENDRITIC SPINE REMODELING IN THE PREFRONTAL CORTEX DURING ALPRAZOLAM WITHDRAWAL

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Benzodiazepine withdrawal is associated with neuroadaptive changes in brain regions involved in emotional regulation, including the prefrontal cortex (PFC). This study examined dendritic spine density and morphology in the prelimbic (PrL) and infralimbic (IL) PFC following alprazolam withdrawal in female Wistar rats. Animals underwent prolonged alprazolam treatment followed by 36- or 96-hour withdrawal. Golgi-Cox staining and quantitative analysis were used to assess spine characteristics. No significant changes in spine density or morphology were observed in the PrL. In contrast, the IL showed significant reductions in branched and mushroom spines, but unchanged overall density. These findings indicate region-specific synaptic remodeling, suggesting selective vulnerability of the PFC during alprazolam withdrawal.

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O-08-P

PHYSICOCHEMICAL CHARACTERIZATION OF SPRAY-DRIED POWDERS ENCAPSULATING PARTHENOLIDE WITH CYCLODEXTRINS

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This study aimed to develop and characterize spray-dried powder formulations of *Tanacetum parthenium* (L.) Sch. Bip. (feverfew) using hydroxypropyl-β-cyclodextrin (HPβCD) as a dual-purpose extraction enhancer and encapsulating agent.

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P *– Food Physical Chemistry*

P-01-P

VOLATILE AND SEMI-VOLATILE COMPOUNDS AND ANTIMICROBIAL PROPERTIES OF CORIANDER SEEDS ESSENTIAL OIL

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Essential oil obtained from coriander (*Coriandrum sativum* L.) seeds was investigated for its volatile and semi-volatile compounds and antimicrobial properties against some common food-born pathogens. According to GC-MS analysis, 14 compounds were identified and quantified in coriander seed oil, representing 96.65% of the total oil. The most abundant compound was β-linalool, representing 50.75% of the total identified compounds, followed by α-pinene (11.53%) and γ-terpinene (9.59%). Significant amounts of *p*-cimene, D-limonene, camphor, geraniol, geranyl acetate were also detected. Concentrations between 0.12 mg/mL and 7.5 mg/mL were tested for antimicrobial properties. The minimum inhibitory concentration (MIC), as well as minimum bactericidal concentration (MBC) of the coriander seeds essential oil were determined by broth microdilution assay against six Gram-positive, six Gram-negative bacterial strains strains and one yeast. The MICs and MBCs ranged from 0.47 mg/mL to 7.5 mg/mL.

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P-02-P

PHYSICO-CHEMICAL PROPERTIES AND PESTICIDE RESIDUES IN DIFFERENT HONEY VARIETIES FROM THE REPUBLIC OF SERBIA

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Honey is a natural bee product traditionally used in human nutrition. The aim of this study was to determine the basic physicochemical characteristics and pesticide content in different types of honey from the territory of the Republic of Serbia. Physicochemical parameters were determined using standard gravimetric and titrimetric methods, while pesticide content was analyzed using dispersive liquid-liquid microextraction (DLLME) in combination with the HPLC-MS/MS method. The obtained results showed that all examined physicochemical parameters were in accordance with the applicable regulations. The most pronounced differences between samples were observed in electrical conductivity, indicating the influence of the botanical and geographical origin of honey. The presence of pesticides was confirmed in three analyzed samples, with acetamiprid and carbendazim identified at concentrations significantly below the maximum permitted values.

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P-03-P

CHARACTERIZATION OF BACTERIAL STRAIN ISOLATED FROM THE TRADITIONAL JAPANESE DISH NATTŌ

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Nattō is a traditional Japanese product made from fermented soybeans, with fermentation carried out by the bacterium *Bacillus subtilis natto,* known for its probiotic potential and ability to synthesize bioactive compounds such as exopolysaccharides. In this paper, the bacterial strain isolated from nattō was characterized in detail to confirm its identity and basic properties. Morphological and biochemical analyses showed that the isolate is a Gram-positive, rod-shaped, aerobic bacterium that is catalase-positive and oxidase-negative. Molecular identification was performed by 16S rRNA gene sequencing and phylogenetic analysis. The obtained sequence showed 99.86% similarity with *Bacillus subtilis subsp. subtilis*, confirming the taxonomic affiliation of the isolate. Considering the previously confirmed ability of *Bacillus subtilis natto* to produce levan, a biocompatible polysaccharide with wide applications, detailed characterization of the microorganism represents a significant step toward its potential use in the food, pharmaceutical, and biotechnology industries.

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P-04-P

THERMAL CHARACTERIZATION OF GRANULATED APPLE POMACE FLOUR BY DSC

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Apple pomace flour (APF) was granulated with different concentrations of zinc sulfate/zinc gluconate and vitamin C as binder, in a fluidized bed process. Seven formulations were produced and characterized by differential scanning calorimetry (DSC). DSC revealed glass transition temperatures (Tg) between 29 and 40 °C, exceeding typical storage temperatures, confirming physical stability of all granulates. Water activity of all samples was below 0.4, consistent with stable dry product quality. Zinc incorporation increased residual mass and shifted cellulose degradation to higher temperatures, indicating enhanced thermal stability through metal-lignocellulose interactions. Samples without vitamin C showed higher Tg values, while added vitamin C reduced Tg due to its hygroscopic nature.

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P-05-P

FTIR-ATR SPECTROSCOPIC DIFFERENTIATION OF MORPHOLOGICAL KERNEL FRACTIONS OF MAIZE HYBRID ZP 707

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Fourier Transform Infrared Spectroscopy with Attenuated Total Reflectance (FTIR-ATR) was used to characterize whole kernel and morphological fractions (endosperm, pericarp and germ) of maize hybrid ZP 707. Spectra were recorded in the 4000-400 cm^{-1} region and analyzed based on characteristic absorption bands. Distinct spectral patterns reflected differences in biochemical composition among kernel tissues. The germ showed pronounced lipid and protein associated vibrations, the endosperm was dominated by polysaccharide related bands typical of starch, while the pericarp exhibited features associated with structural cell wall polysaccharides. The whole kernel spectrum represented an integrated response of all fractions. Results confirm that FTIR-ATR spectroscopy enables rapid and reliable differentiation of maize kernel tissues based on their molecular composition.

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Q *–Physico-Chemical Analysis*

Q-01-P

A MODIFIED XPS ATTENUATION MODEL FOR NON-UNIFORM DOPANT INCORPORATION IN GD-DOPED Γ-Fe_2O_3 NANOCLUSTERS

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This paper proposes an XPS-based model for calculating the effective modification depth of Gd-doped γ-Fe_2O_3 nanoflower clusters. The idea is based on overlayer and core-shell models using XPS intensities to quantify the attenuation of core signal, which can be used to calculate the thickness of the overlayer. An island growth approach was used to approximate the attenuation caused by non-uniform dopant incorporation. Simple attenuation equations were modified with an additional structural term to better describe the experimental curve. An effective modification depth was calculated to be 0.89 nm, with substantial uncertainty (± 0.41 nm), reflecting the limited dataset. These results demonstrate that XPS-based modeling can provide useful insights into surface modification in complex nanostructured systems, although further experimental data are required to improve quantitative reliability. The model is motivated by previously observed surface-specific changes in Gd-doped γ-Fe_2O_3, where XPS revealed defect formation and redox variations localized near the nanoparticle surface.

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Q-02-P

REFINEMENT OF THE *T–x* DIAGRAM OF THE In – Se SYSTEM

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The aim of the present work was the verification of the phase diagram of the In–Se system over the composition range from 15.0 to 63.4 mol.% Se, as well as the determination and confirmation of the structures of the principal intermediate phases in this system. By employing the differential thermal analysis method, the *T–x* diagram of the In–Se system in the range from 15.0 to 63.4 mol.% Se has been refined. Furthermore, it has been demonstrated that two modifications of In_6Se_7, which are very close in both composition and structure, coexist. At least three structures stable in different temperature ranges have been found to correspond to the stoichiometry In_2Se_3. It has been established that the high-temperature modification δ-In_2Se_3 possesses a structure similar to that of defect wurtzite.

R *– Photochemistry, Radiation Chemistry, Photonics*

R-01-P

APPLICATION OF DIGITAL HOLOGRAPHIC MICROSCOPY IN REAL-TIME POLLEN TUBE GROWTH MONITORING

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This study presents the application of digital holographic microscopy to real-time imaging of pollen grains and pollen tube growth. This method is non-destructive and enables continuous monitoring of pollen germination and tube elongation without staining. We investigated the germination of forest violet pollen. Our results demonstrate digital holographic microscopy as a powerful, label-free tool for studying transparent biological samples and dynamics in real-time.

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R-02-P

ADSORPTION AND REDUCTION OF METHYLENE BLUE IN A PLASMONIC ENHANCED PHOTOCATALYTIC MICROREACTOR

Olga Jakšić, Katarina Radulović, Marko Bošković, Marko Obradov, Olivera Živković, Katarina Cvetanović, and Dana Vasiljević-Radović

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We present a coupled electromagnetic and kinetic simulation of a plasmonic photocatalytic microreactor in which Methylene Blue (MB) undergoes adsorption, desorption, and photoreduction to Leucomethylene Blue (LMB) on an Au-Si substrate. A lateral probe beam through the Pyrex cell yields time-resolved absorbance, reflectance, and transmittance spectra (400–800 nm) via the Transfer Matrix Method applied to the full Air–Pyrex–Solution–Pyrex–Air stack, while a vertical beam provides a surface plasmon resonance read-out of interfacial adsorption dynamics. The solution dielectric function is obtained from Maxwell Garnett effective medium theory, with MB described by a three-term Lorentzian oscillator model and LMB permittivity approximated as that of water. The SPR signal cleanly resolves the initial rapid adsorption of MB onto gold upon solution introduction, the slower competitive dynamics during illumination as surface-bound MB is reduced and released as LMB, and any re-adsorption of re-oxidised MB during the dark phase.

Acknowledgment
This research has been financially supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No. 451-03-136/2025-03/200026) and by the Science Fund of the Republic of Serbia, Grant No. 7451, Plasmonic-based light harvesting for photocatalytic microfluidic devices – PlasmaHarvest.

S *– Free Topic*

S-01-O

BACTERIAL RESILIENCE AND DISPERSAL IN DYNAMIC OXYGEN GRADIENTS

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Oxygen availability is a central environmental cue for aerobic bacteria, but the response of surface-associated populations to oxygen landscapes that change in space and time remains poorly resolved. We developed a single-layer microfluidic platform combining membrane-separated gas-exchange serpentines with a 20 × 4 × 0.1 mm observation chamber. Analytical modelling, COMSOL simulations, and ruthenium-based oxygen imaging quantified exchanger performance and chamber-wide concentration fields. Single-cell imaging of *Pseudomonas putida* KT2440 during a homogeneous oxygen downshift and reversal of a spatial gradient showed that populations maintained exponential growth for several generations after a decrease from 100% to 1% air saturation. This growth-inertia period preceded cell shortening, microcolony disaggregation, and detachment. Gradient reversal then produced preferential attachment and compact microcolonies in the newly oxygen-rich region, while the oxygen-poor region developed elongated chains and lost surface-associated cells. The delayed response is consistent with transient metabolic buffering or physiological memory and generates coexisting “settler” and “disperser” subpopulations.

Acknowledgment. This work received funding from the European Union Horizon 2020 programme under Marie Skłodowska-Curie Grant Agreement No. 956457 (COPERMIX) and from the Swiss National Science Foundation PRIMA Grant No. 179834.

S-02-P

PORTUGIESER WINE POMACE: SCREENING OF BIOACTIVE COMPOUNDS AND ANTIMICROBIAL POTENTIAL AGAINST ORAL ISOLATES

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Wine pomace is the residue of pressed grapes from wine production. The objective of this research was to investigate the Portugieser wine pomace extract (WPE) phenolic profile and antimicrobial potential against oral isolates and reference strain. Detection of sustainable antimicrobials supports the manufacturing of numerous value-added products. According to RP-HPLC analysis seven compound were identified and quantified in WPE. Predominant compound was catechin (635.33±2.08 μg/g dry weight (DW)), followed by *trans*-cinnamic acid (283.33±22.28 μg/g DW), gallic acid (121.00±1.73 μg/g DW), naringenin (59.33±5.69 μg/g DW), *p*-coumaric acid (27.33±0.58 μg/g DW), *trans*-ferulic acid (9.57±1.19 μg/g DW) and hesperetin (2.67±0.38 μg/g DW). The minimum inhibitory concentration (MIC) was determined on following bacterial strains: *Staphylococcus aureus* ATCC BAA-1026, and oral isolates, *Streptococcus mitis* and *Streptococcus mutans* (MIC=2.81 mg/mL; MIC=2.34 mg/mL; MIC= 2.81 mg/mL, respectively).

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This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (grant no 451-03-33/2026-03/200051, 451-03-33/2026-03/200178, 451-03-34/2026-03/200178, 451-03-33/2026-03/200017; 451-03-33/2026-03/200175). M.T. was supported by the 2025-1.2.4-TÉT-2025-00033 project.

S-03-P

EVALUATION OF CYTOTOXIC EFFECTS OF MICROPLASTIC PARTICLES IN HUMAN LUNG FIBROBLAST - IN VITRO STUDY

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Microplastic particles (MPs) are ubiquitous pollutants smaller than 5 mm and their increasing detection in various human tissues has raised concerns about their potential adverse effects on human health. This study examined early and late cytotoxic effects of polyethylene terephthalate (PET) MPs in human MRC-5 fibroblasts *in vitro*. Cells were incubated with increasing concentrations of MPs for 24 h. Early cytotoxicity was assessed by 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay immediately post-treatment, while late effects were examined via colony formation assay two weeks later. Results showed that MRC-5 cells viability decreased 24 h post-treatment compared to the control without significant differences among experimental groups. Clonogenic survival revealed that proliferative capacity declines concentration-dependently under higher MPs doses. Our findings suggest that treatment with MPs can possibly lead to accumulation of adverse effects in MRC-5 cells.

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S-04-P

PRENATAL EXPOSURE TO EXTREMELY LOW-FREQUENCY ELECTROMAGNETIC FIELDS ALTERS ECTONUCLEOTIDASE ACTIVITY IN THE DEVELOPING RAT HIPPOCAMPUS

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Exposure to extremely low-frequency electromagnetic fields (ELF-MF) has increased with technological development and is a potential environmental factor affecting brain development. Ectonucleotidases (NTPDase/eN) and adenosine deaminase (ADA) regulate extracellular nucleotide and nucleoside levels, modulating purinergic signaling involved in neuronal proliferation, differentiation, and synaptogenesis. In this study, we investigated the activities of these enzymes in the developing hippocampi of male rat offspring following prenatal ELF-MF exposure (0.5 mT 50 Hz). Prenatal ELF-MF exposure significantly decreased ATP, ADP, and AMP hydrolysis compared to controls, indicating reduced NTPDase/eN activity and potential disruption of extracellular nucleotide metabolism. In contrast, ADA activity remained unchanged, suggesting adenosine degradation was unaffected. These findings demonstrate that prenatal ELF-MF exposure selectively modulates purinergic signaling in the developing hippocampus, which may contribute to altered synaptic function and neurodevelopmental outcomes.

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S-05-P

PRENATAL VALPROIC ACID EXPOSURE SELECTIVELY REDUCES HIPPOCAMPAL ADP HYDROLYSIS WITH LIMITED MODULATION BY MATERNAL FLAXSEED OIL SUPPLEMENTATION

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This study examined the effects of prenatal valproic acid (VPA) exposure and maternal flaxseed oil (FSO) supplementation on hippocampal ectonucleotidase activity in female rat offspring. Eight Wistar dams were divided into Control, FSO, VPA, and FSO+VPA groups and female offspring were analyzed at postnatal days 28–30. ATP, ADP, and AMP hydrolysis as functional indicators of ectonucleotidase activity were measured in hippocampal membrane fractions. Two-way ANOVA showed significant VPA effects on all substrates, with no FSO or interaction effects. Post hoc analysis

revealed reduced ADP hydrolysis in the VPA group ($p < 0.05$), while ATP and AMP were unchanged. The FSO+VPA group showed intermediate, non-significant values, suggesting limited FSO modulation. Overall, prenatal VPA selectively impairs ectonucleotidase activity, mainly reducing ADP hydrolysis.

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S-06-P

GLuN2A SUBUNIT MODULATES CD39/CD73 ACTIVITY IN LIPOPOLYSACCHARIDE -INDUCED NEUROINFLAMMATION IN MICE

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Lipopolysaccharide (LPS)-induced inflammation overstimulates N-methyl-D-aspartate receptors (NMDARs), disrupting glutamatergic signaling. Neuroinflammation also increases extracellular ATP and adenosine, overactivating purinergic pathways. The ectonucleotidases CD39 and CD73 regulate this balance by converting ATP to adenosine. This study examined the role of GluN2A subunit in modulating CD39/CD73 activity under LPS conditions. Using wild-type (WT) and GluN2A knockout (KO) mice, nucleotide hydrolysis was measured in cortical and hippocampal synaptosomal fractions. LPS increased CD39/CD73 activities in the cortex of WT mice, indicating enhanced ATP breakdown. In contrast, KO mice showed reduced basal ATP/ADP/AMPase activities and no significant LPS response, except a slight decrease in hippocampal ATP hydrolysis. These findings suggest that LPS enhances purinergic metabolism mainly in the cortex, while GluN2A absence prevents enzymatic changes, highlighting its role in neuroinflammation and synaptic stability.

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S-07-P

CONTENTS OF SOME MINERALS IN DANDELION ROOTS OF WASTERN SERBIA

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The root of *Taraxacum officinale* (dandelion) contains numerous beneficial compounds and elements, but also those that may be harmful to human health. In this study, five elements (K, Na, Ca, Mg and P) were determined in the roots of dandelion. During the autumn of 2022, dandelion root samples were collected from nine locations in the area of the municipality of Ljubovija, in Western Serbia. Samples were prepared by using dry digestion in triplicate, and the ash was dissolved in 6M HCl, followed by dissolution in 0.1M HNO_3. The content of the elements in the dandelion roots was determined using inductively coupled plasma optical emission spectroscopy (ICP-OES). The obtained results indicated content of investigated elements grows in following order: Sodium (Na) < Magnesium (Mg) < Calcium (Ca) < Phosphorus (P) < Potassium (K). In addition, the mutual relations of elements that are important in determining nutritional interrelationships were calculated.

Acknowledgment
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S-08-P

NLP-BASED CROSS-MATRIX ANALYSIS OF METABOLOMICS DATA IN DEPRESSION

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Depression is a prevalent psychiatric disorder with a complex multifactorial etiology and low remission rates. To better characterize its biochemical background, we applied natural language processing-based text-mining approach using the MetaboListem algorithm to systematically analyze depression-related metabolomics studies in blood and hippocampus (HIPP). The analysis included 730 and 226 preclinical and clinical studies, identifying 1493 and 530 distinct metabolite alterations in blood and HIPP, respectively. Pathway enrichment analysis (MetaboAnalyst v6.0) revealed consistent dysregulation of amino acid metabolism, primarily, across both matrices. Overall, depression is associated with consistent disruptions in amino acid metabolism across both the circulation and HIPP.

Acknowledgment
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S-09-P

MATRIX-DEPENDENT DIFFERENCES IN MALDI-MS LIPID DETECTION IN BIOLOGICAL SAMPLES USING DHB AND 9-AA

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Although Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry (MALDI-MS) offers rapid lipid profiling, its analytical success can be significantly influenced by the choice of matrix. This study compared the effects of 2,5-dihydroxybenzoic acid (DHB) and 9-aminoacridine (9-AA) on lipid detection from human plasma extracts analyzed in positive ion mode. Lipids were isolated using a modified Folch method and analyzed under identical acquisition conditions. DHB showed superior signal intensity and broader coverage of complex phospholipid profiles compared to 9-AA. Specifically, phosphatidylcholine (PC) and lysophosphatidylcholine (LPC) species were more consistently detected with DHB, leading to higher and more variable PC/LPC ratios whereas 9-AA exhibited significantly lower sensitivity toward these choline-containing lipids. Our findings emphasize that matrix selection is a decisive factor in lipidomics, directly impacting the reliability and depth of the resulting molecular profiles.

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S-10-P

LIGAND-DEPENDENT BIOLOGICAL RESPONSES TO SURFACE-MODIFIED TiO_2 NANOPARTICLES

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Titanium dioxide nanoparticles (TiO_2 NPs) have numerous industrial, environmental, and biomedical applications due to their unique properties. However, their high surface reactivity, tendency for agglomeration, and ability to induce oxidative stress and inflammation across various cells and tissues continue to raise safety concerns. Although surface modification strategies are used to mitigate TiO_2 NPs toxicity, their safety profiles remain inconsistent. Our current study evaluates the mechanisms governing surface-modified TiO_2 NPs' behavior in diverse biological systems through literature analysis combined with our original experimental findings on splenic response. Results indicate that while surface modifications can improve stability and reduce toxicity, these effects might be organ-specific and strongly depend on the chemical nature of the modifying agent. This underscores the necessity for mandatory multi-organ and -cell assessments to ensure the development of truly safer nanomaterials.

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S-11-P

EXTRACTION AND CHARACTERIZATION OF IRREGULAR POLYSTYRENE MICROPLASTIC PARTICLES FOR BIOLOGICAL RESEARCH

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Microplastic particles (MPs), smaller than 5 mm in diameter, are a well-known pollutant and a potential risk to human health. MPs originate either from industrial production (primary MPs), or from the breakdown of larger plastic waste (secondary MPs). In order to obtain MPs true to those found in the environment, we generated polystyrene (PS) particles using the mechanical abrasion method. The resulting heterogeneous fragments were characterized, and their chemical composition was confirmed using multiple analytical techniques. The presented data suggests that this methodology is a promising alternative to commercially available MPs, while the irregularly shaped particles provide a more realistic and representative model of naturally occurring MPs. Further research should focus on the potential toxicity of obtained polymers in *in vitro* and *in vivo* models.

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S-12-P

DOSE-DEPENDENT EARLY RENAL DYSFUNCTION FOLLOWING ACUTE MICROPLASTIC EXPOSURE IN MALE RATS

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Microplastic particles smaller than 5 mm (MPs) are widespread environmental contaminants with potential adverse biological effects. This study evaluated the acute effects of in-house produced irregular polyethylene terephthalate (PET) MPs administered orally as a single dose (1.4 or 35 mg/kg) in male Wistar rats. Renal function was assessed 24 h post-exposure via urinary and serum biochemical parameters. In urine, compared to control, pH was elevated by 22% in the higher-dose treated group, while protein levels only showed an increasing trend. Specific gravity remained unchanged and no hematuria was detected, suggesting preserved concentrating ability and no mechanical damage. Serum analysis revealed significant increases in urea (by 43 %) and creatinine (by 37 %) levels in the higher-dose treated group relative to the control, indicating impaired renal function. These findings suggest that even a single exposure to MPs may affect renal health.

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This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants No. 451-03-33/2026-03/200017 and 451-03-33/2026-03/200175).

S-13-P

AI-ASSISTED METHODOLOGY FOR STRUCTURAL SHIELDING DESIGN AND EVALUATION OF MEDICAL DIAGNOSTIC X-RAY FACILITIES

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This paper presents a methodology for the calculation of shielding barriers in medical facilities where radiation practices in the field of diagnostic medical X-ray imaging are performed. The methodology is based on radiation protection principles, computational workflow standardization, and support assisted by the Anthropic Claude large language model (LLM). The methodology and the associated computational skill were developed for conventional X-ray diagnostics, fluoroscopy, computed tomography, mammography, dental X-ray diagnostics, and interventional procedures. The methodology integrates shielding design principles derived from NCRP, ICRP, and IAEA

recommendations together with the Serbian regulatory framework. Particular emphasis is placed on standardized parameter acquisition, conservative uncertainty treatment, barrier transmission calculations, assessment of occupancy factors, workload assessment, and traceability of technical documentation.

S-14-P

QUERCETIN AND ROOPEROL AS DIRECT RADICAL SCAVENGERS - A DFT STUDY

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Two natural catecholic compounds, quercetin and rooperol, were studied in silico in order to understand their radical scavenging potency. To that purpose, estimation of H-atom donation to $CH_3OO^{\bullet}$ and $HOO^{\bullet}$, thermodynamics, kinetics and tunnelling, three forms of chemical reaction control, were theoretically performed (Gaussian 09, DFT, M05-2X, 6- 311++G(d, p)). The influence of pentyl ethanoate and water was calculated using SMD solvation model. For calculations regarding rate constants of studied reactions, Eyringpy program was used. Obtained results indicate that in lipid media, H-atom donation from catecholic OH groups of quercetin via PCET is more relevant than from C-ring enolic moiety. Also, H-atom donation from A-ring OH groups of rooperol is determined to be favoured. Namely, allylic hydrogens of rooperol are poorly abstractable via HAT. Obtained results for aqueous environment indicate the 3-O^{-} phenoxide anion of quercetin and 4′-O^{-} phenoxide anion of rooperol as preferred sites for $CH_3OO^{\bullet}$ and $HOO^{\bullet}$ inactivation via SET. Results of the performed kinetic analysis confirm the traditional view that phenolic OH groups play a central role in radical scavenging by polyphenols.

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T *– Education, History*

T-15-P

ANDRE GEIM

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Andre Geim is known for his research in the field of graphene and materials science. Together with Konstantin Novoselov, he discovered and isolated single-layer, two-dimensional graphene. Among his scientific achievements is the so-called Gecko tape, whose surface is covered with numerous fine hairs, whose total Van der Waals force achieves the tape's super stickiness. He received the Nobel Prize in Physics and the Ig Nobel Prize.

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In memory of PhD Tibor Halaši (1949-2024), Teacher at Faculty of Science, Department of Chemistry, Biochemistry and Environmental Protection, Methods of Teaching Chemistry, History of Chemistry, University of Novi Sad.

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