



Society of Physical Chemists of Serbia

PHYSICAL CHEMISTRY 2021

*15th International Conference on
Fundamental and Applied Aspects of
Physical Chemistry*

PC2021

The Conference is dedicated to the

30th Anniversary of the founding of the Society of Physical Chemists of Serbia

and

100th Anniversary of Bray-Liebhaafsky reaction



PHYSICAL CHEMISTRY 2021

15th International Conference on Fundamental and Applied Aspects of Physical Chemistry

Organized by

The Society of Physical Chemists of Serbia (SPCS)



in co-operation with

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Boreskov Institute of Catalysis, Siberian Branch of Russian Academy of Sciences



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PL- Plenary lecture

01-PL**DISSIPATIVE STRUCTURES AND BIOLOGICAL RHYTHMS**

Albert Goldbeter

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Sustained oscillations abound in biological systems. They occur at all levels of biological organization over a wide range of periods, from a fraction of a second to years, and with a variety of underlying mechanisms. They control major physiological functions, and their dysfunction is associated with a variety of physiological disorders. The goal of this presentation is (i) to give an overview of the main rhythms observed at the cellular and supracellular levels, (ii) to briefly describe how the study of biological rhythms unfolded in the course of time, in parallel with studies on chemical oscillations, (iii) to present the major roles of biological rhythms in the control of physiological functions, and (iv) the pathologies associated with the alteration, disappearance, or spurious occurrence of biological rhythms. Among the rhythms discussed are neural and cardiac rhythms, metabolic oscillations such as those occurring in glycolysis in yeast, intracellular Ca^{++} oscillations, cyclic AMP oscillations in *Dictyostelium amoebae*, the segmentation clock that controls somitogenesis, pulsatile hormone secretion, circadian rhythms which occur in all eukaryotes and some bacteria with a period close to 24h, the oscillatory dynamics of the enzymatic network driving the cell cycle, and oscillations in transcription factors such as NF- κ B and tumor suppressors such as p53. The concept of dissipative structures applies to temporal oscillations and allows us to unify within a common framework the various rhythms observed at different levels of biological organization, regardless of their period and underlying mechanism.

02-PL**SYNCHRONISATION OF GLYCOLYTIC ACTIVITY IN
YEAST CELL POPULATIONS**

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Glycolysis is the central metabolic pathway of almost every cell and organism. We report on glycolytic oscillations of intact yeast cells at the level of the cell population as well as at the level of individual cells. Synchronisation depends on the cell density of a population, because the collective oscillatory behaviour of a yeast cell population ceases when the cell density of the population falls below a threshold. At high cell densities, the dynamics is oscillatory, but below a critical density the collective dynamics becomes quiescent. Whereas cells in stirred cell suspension ceased to oscillate, immobilized cells were found to show glycolytic oscillations, even at very low cell densities. This means, the transition between oscillatory and stationary dynamics in immobilized or suspended cells follows different phase types of transitions.

The pathway to synchrony of originally quiescent, immobilized cells was achieved by a the synchronisation of the frequencies of the cellular oscillations, which was followed by a synchronisation of their phases. The pathway leading to synchronisation involved a narrowing of the frequency distribution in conjunction with a shift in the mean frequency of the glycolytic oscillations to larger values. The population was entrained by those cells that oscillated at higher frequencies; this is typical for synchronisation due to phase advancement.

Two spatial aspects of self-organization observed in extended populations of immobilized yeast cells were addressed: (1) the emergence of regional clusters and (2) the emergence of travelling waves of glycolytic activity. Although the cells were either completely or partially synchronised, travelling glycolytic waves arise due to a phase difference in space. These waves propagated though the field of view; however, the intracellular dynamics of each cell is homogeneous in space, due to the small diameter of the cell.

03-PL**MAKING NON-BIOCHEMICAL ARTIFICIAL LIFE IN A TEST TUBE**Juan Perez-Mercader^{1,2}

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Living systems on Earth are broadly characterized as complex chemical systems capable of concomitantly (i) process information, (ii) metabolize (including making their own parts from simpler components), (iii) self-reproduce and (iv) evolve. These properties are traditionally associated with the presence in extant living systems of three common universal and interdependent features: the existence of a membrane boundary, metabolism and information-carrying molecules. For each of these there exists an origins-of-life school of thought positing that one of them preceded the others in the path from non-life to proto-life to life. However, their interconnectedness makes exploring any of the three in the absence of the rest extremely difficult.

Notwithstanding the above, we show that properties (i) through (iv) can be described by a small set of unifying equations whose solutions, remarkably, display the above properties. Inspired and guided by these solutions, we present progress in the area of life's origins and its chemical synthesis resulting from experiments on autonomous system boot-up during the chemically controlled non-equilibrium self-assembly of functional, non-biochemical and small molecule-based polymeric vesicles. We follow their dynamical evolution with membrane growth and metabolism working in concert under autonomous chemical control. All this is achieved by implementing a PISA (Polymerization Induced Self-Assembly) polymerization/encapsulation scenario in an aqueous medium, which solves the concentration problem and generates an all-important free-energy gradient which provides the necessary boot-up conditions for these fully artificial systems. By design, our 1-pot chemical system ("test tube") uses reversible addition-fragmentation-chain transfer (RAFT) polymerization and completely avoids bio-chemistry. We monitor the consequences of the on-going active amphiphilic block copolymer synthesis with their resulting molecular self-assembly and evolution using electron and optical microscopy. (We will present actual microscope movies of the resulting active vesicles and their population.) We find that this dissipative self-assembly process leads to vesicles with diameters between 0.5 and 10's of microns which exhibit several emergent, life-like, properties. These include periodic growth and partial collapse, system self-reproduction, together with homeostasis, competition and phototaxis at the population level. We will briefly discuss the extension of the above by executing the PISA process with oscillatory chemical reactions which are actually able to compute as chemical Turing machines and control the assembly sequence and time evolution of their self-generating, entrapping and self-replicating vesicles. Taken together these results offer insights into artificial life, as well as into the formation of small-molecule protocells an route to the earliest living systems on the Earth as precursors to extant life and biochemistry.

04-PL

**DESIGN OF A PHOTOCROMIC OSCILLATOR TO BE USED AS
DYNAMICAL MODEL OF PACEMAKER NEURONS**

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Neuromorphic engineering implements surrogates of neurons to develop Artificial Intelligence. A strategy to devise artificial neuron models is to use non-linear chemical systems that can mimic neural dynamics. This work presents the design of a new photochemical oscillator to be used as a dynamical model of pacemaker neurons. Such photochemical oscillator is based on two photochromic compounds. The spectral and kinetic features required to have oscillations are presented rigorously using numerical integration of non-linear differential equations. The designed artificial pacemaker neuron can communicate with other chemical neuron models through the transmitted and/or emitted light.

05-PL**NUCLEOPEPTIDE NETWORKS OUT-OF-EQUILIBRIUM**

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Many fundamental cellular functions, including replication and translation, involve synergistic activity between nucleic acids and proteins/peptides. Yet, studies with synthetic replicators have focused largely on the activity of each class of these molecules separately. We show here that short nucleopeptide chimeras can replicate through autocatalytic and cross-catalytic processes, governed synergistically by nucleobase hybridization and the assembly of peptide segments. Remarkably, within small networks of complementary nucleopeptides, unequal replication kinetics induces clear selectivity toward the formation of a certain species. The selectivity may be maximized to almost extinction of the weakest replicator when the system operates far from equilibrium and manipulated through changes in the physical and chemical conditions.[1] We will discuss how similar processes may have led to the emergence of the first functional nucleic-acid-peptide assemblies prior to the origin of life.

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06-PL**COMPETITIVE ADSORPTION AND SELECTIVITY ASPECTS OF CARBON DIOXIDE, WATER VAPOUR, NITROGEN, AND SULFUR DIOXIDE ON ACTIVATED CARBON FOR CAPTURE FROM FLUE GASES****Mark Thomas**

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There is extensive interest in post combustion flue gas treatment for mitigating CO₂ emissions and removal of acid gases. Adsorption on porous materials is a potential low energy method for capturing CO₂. In recent years, many novel porous materials have been synthesized. However, the knowledge of selectivity and competitive adsorption of complex mixtures on porous materials remains superficial. In this study we investigate the adsorption of the main flue gas components (CO₂, N₂, SO₂, and water vapour) on Filtrasorb 400 activated carbon in order to understand adsorption characteristics of the main flue gas components and competitive adsorption effects. The adsorption isotherms of the pure components of flue gas CO₂, N₂, SO₂ and H₂O vapour were investigated. The isosteric enthalpies of adsorption were determined as a function of surface excess. The enthalpies at zero surface coverage have the order: SO₂ > H₂O > CO₂ > N₂. However, the SO₂ isosteric enthalpy decreases with increasing surface excess and is lower than that of water vapour at high surface excess uptake values. The temperature range for CO₂ adsorption covers the subcritical to supercritical gas transition. There was no evidence for isosteric enthalpy differences over this temperature range. The adsorption kinetics for SO₂ and H₂O adsorption were measured for each isotherm pressure increment. In both cases the adsorption kinetics followed the linear driving force model. The adsorption mechanisms for both SO₂ and H₂O kinetic trends are discussed in terms of the adsorption mechanisms. The water vapour adsorption kinetics showed a minimum in the region where water molecules form clusters around functional groups, which merge in the pores. The SO₂ adsorption kinetics also show a minimum with increasing surface coverage and this is attributed to dipole-dipole interactions. The activation energies for diffusion of both SO₂ and H₂O into F400 were very low. The adsorption kinetics of both pure N₂ and CO₂ were too fast to be measured accurately by the gravimetric method used in this study. Ideal Adsorbed Solution Theory (IAST) was used to calculate competitive adsorption of SO₂/CO₂ and CO₂/N₂ from the isotherms of the pure components. In the case of CO₂/H₂O adsorption, the adsorption mechanisms of H₂O and CO₂ are different and therefore, IAST was not applicable. The competitive adsorption of CO₂/N₂ was investigated using the Integral Mass Balance (IMB) experimental method and this was used for validation of the IAST. The competitive adsorption of CO₂/H₂O is the most important for CO₂ capture and this was also investigated using the IMB method. The results show that both thermodynamic and kinetic effects are important. The results provide an insight into the role of competitive adsorption in the capture of CO₂ and SO₂ from flue gases by adsorption on porous materials from both thermodynamic and kinetic perspectives.

07-PL

FUNCTIONAL BIODYNAMICS: THE YIN COMPLEMENT

Jochen Mau

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A previous paper elaborated on holistic functional dynamics of human-body system with assumptions about “driving forces” of physiological processes from a phenomenological viewpoint. At the behavioral level of person’s operations in body’s outside world, in particular in interaction with other persons in society, motivations had been considered in more detail though still without attempts to expand the mathematical model accordingly

08-PL**COILED-COILS FOR THE DESIGN OF CELLULAR LOGIC CIRCUITS
AND NEW PROTEIN FOLDS**

Roman Jerala

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Coiled-coil (CC) dimers are ubiquitous building modules in natural proteins. Rules that defined interactions in CC dimers are relatively well known which allows us to design new CC dimers with selected stability and selectivity. Although CC dimers have been known since Francis Crick, recently their application in cell regulation and construction of new building modules are experiencing an explosive growth. We have designed new CC pairs that can be fused to and incorporated into other proteins, that enables new type of regulation of biological processes with increased response and fast kinetics (1,2).

CC dimers can be concatenated into longer chains which enables construction of new modular protein folds based on topological principles distinct from natural proteins. Coiled-coil protein origami (CCPO) have interesting properties and we are designing new modalities of their construction that enable multiple use of the same building modules and design of the folding pathways and other properties (3-6).

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09-PL**HYBRID ORGANIC-INORGANIC PEROVSKITES**

Alessandro Stroppa

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Hybrid Organic-Inorganic Perovskites (HOIPs) are introducing new directions in the materials science landscape. In this talk, we will discuss the intriguing origin of ferroelectricity in HOIPs. In particular, we highlight the hybrid improper mechanism where Jahn-Teller cooperative distortions are subtly coupled to inversion symmetry breaking giving rise to a switchable electric polarization. Symmetry invariants theory permits to predict a magneto-electric coupling which has been recently confirmed by experiments. We propose further examples of the complex multifunctional behaviour arising from the organic and inorganic dual nature as well as from the interplay between ferroelectricity and spin-related properties in hybrid perovskites. In particular we discuss a recently synthesized ferroelectric layered two-dimensional HOIP, i.e. (AMP)PbI₄ (AMP=4-aminomethyl-piperidinium). We report a new effect, i.e., an extraordinarily large Rashba anisotropy that is tunable by ferroelectric polarization: as polarization is reversed, not only the spin texture is inverted, but also the major and minor axes of the Rashba anisotropy ellipse in k-space are interchanged, i.e. a pseudo-rotation. A $k \cdot p$ model Hamiltonian and symmetry-mode analysis reveal a quadrilinear coupling between the cation-rotation modes responsible for the Rashba ellipse pseudo-rotations, the framework rotation, and the polarization.

10-PL**ANTITUMOR DRUGS IMMOBILIZED INTO MESOPOROUS SILICA SBA-15**

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Conventional therapeutics, such as cisplatin, beside their benefit effects in fight against cancers confronts quite a few challenges [1]. The main goals of chemotherapeutics are to hinder the tumor expansion, reduce growth of tumor cells and increase the patient's survival period. Cisplatin alone or in combined therapy is a first-line agent for several cancers (e.g. testicular, ovarian, lung, head and neck tumors). However, its antitumor efficiency is limited due to dose-dependent toxicities (e.g. nephro- and neurotoxicities) and intrinsic or acquired cellular resistance [2].

Silica-based materials are already highly promising candidates in several fields of medicine including cancer therapy [3,4]. The rationale of loading of highly active anticancer compounds into particles lie in the following: prevention of hydrolysis and accumulation in the healthy tissues/organs, tailorable drug release, as well as local application in tumor tissues in high doses.

SBA-15 or its functionalized forms potentiate and modify mechanism of action of metal-based (e.g. cisplatin, ruthenium(II), organotin(IV) compounds) or natural occurring compounds (e.g. emodin) [3-9]. For instance, SBA-15 loaded with cisplatin induced senescence in survived clones of B16F10 mouse melanoma cells [3]. SBA-15 grafted with $\text{Ph}_3\text{Sn}(\text{CH}_2)_6\text{OH}$ triggers apoptosis in B16 cells followed by the development of a nonproliferative melanocyte-like phenotype of surviving cells [5]. Moreover, same nanomaterial almost completely abolished tumor progression *in vivo* in melanoma syngeneic C57BL/6 mouse model without visible side effects. $\text{Ph}_3\text{Sn}(\text{CH}_2)_3\text{OH}$ loaded into SBA-15 reduces metastatic potential of highly invasive serous ovarian carcinoma A2780 cells [6]. Importantly, functionalization of SBA-15 has an influence on the mode of action and differentiation inducing properties [7]. SBA-15 potentiates action of $[\text{Ru}(\eta^6\text{-}p\text{-cymene})\text{Cl}_2\{\text{Ph}_2\text{P}(\text{CH}_2)_3\text{SPh-}\kappa\text{P}\}]$ and emodin against B16 cells [8,9]. These approaches present a safer mode in tumor treatment compared to induced apoptosis alone.

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11-PL

CEREBRAL HYPOPERFUSION AND PROGESTERONE TREATMENT ALTER PARAMETERS OF OXIDATIVE STRESS AND ANTIOXIDANT DEFENCE IN MALE RATS

I. Guševac Stojanović¹, A. Todorović¹, S. Pejić¹, N. Tatalović², D. Blagojević², J. Martinović¹, I. Grković¹, N. Mitrović¹, M. Zarić¹, and D. Drakulić¹

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Numerous natural compounds, like progesterone (P4), a sex steroid hormone, are highlighted as promising agents for treatment of different disorders including prolonged disturbance of blood flow. However, its action on several oxidative stress markers (pro/antioxidant balance, products of lipid peroxidation and phosphatidylcholine to lysophosphatidylcholine intensity ratio) and one of the major components of antioxidant system, superoxide dismutase in rat prefrontal cortex (PFC) following permanent bilateral occlusion of common carotid arteries (2VO) is not completely investigated. According to the obtained results, levels of investigated oxidative stress markers and SOD activity were altered in 2VO animals treated with vehicle, while P4 treatment returned them to control values. Overall, presented data indicate that P4 might manifest antioxidative features in PFC of 2VO rats.

12-PL

**SELF-CREATION OF COMPLEX CHEMICAL ENTITIES THAT CREATE
COMPLEX CELLS, GROWING AND FORMING UNUSUAL STRUCTURES,
MOVEMENTS AND MACHINES THAT CAN SWITCH ITSELF TO
ANOTHER**

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First Law of Thermodynamic describe that everything cannot be -self creator or destroyed in an isolator system. In open systems far from thermodynamic equilibrium. However, they exist systems that exist far from Thermodynamic Equilibriums that are supplied by chemical systems and continuously moving father from equilibrium. They are building chemical cells that can take compounds from outside, react and one compound will stay inside and next move outside. May create very complex towers. Machines cand move in different ways and may produce different complex structures. It is the basic Law of Chemical Self-creation.

A - Chemical Thermodynamics

A-01-P

THERMODYNAMIC PROPERTIES OF PURINE

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In the present work the temperature dependence of the molar heat capacity for purine CAS 120-73-0 has been measured for the first time over the temperature range from 5 K to 350 K and $p = 0.1$ MPa by the precision adiabatic vacuum calorimeter. Based on the experimental data, the thermodynamic functions of the sample have been determined for the range $T = (0 - 350)$ K. Using combination of the adiabatic and combustion calorimetry results the thermodynamic functions of formation of purine at $T = 298.15$ K and $p = 0.1$ MPa have been calculated. The low-temperature X-ray diffraction was used for the determination of sample thermal expansion coefficients.

A-02-P

LOW-TEMPERATURE STUDIES OF AURIVILLIUS PHASE $\text{Bi}_5\text{Ti}_3\text{MnO}_{15}$

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Manganese-containing multiferroic Aurivillius layered perovskite was synthesized and characterized by XRD and XRF. The obtained compound is isostructural to its ferrous analog. Second order insulator-metal phase transition was detected at 126 K using low-temperature XRD and DSC. Heat expansion of the material was studied in the temperature range of 80-400 K.

A-03-P

CONTRIBUTION OF DIFFERENT INTERACTIONS TO THE EXCESS GIBBS ENERGY OF MIXING IN AQUEOUS ELECTROLYTE SOLUTIONS

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The thermodynamic properties of the mixed electrolyte solutions are conveniently described in terms of excess quantities. The excess Gibbs energy of mixing, presents the difference between the excess free energy of a mixed electrolyte solution and free energies of the individual binary electrolyte solutions at the same temperature, pressure and total ionic strength. In this paper the excess Gibbs energy of mixing is calculated for series of mixed electrolyte solutions and possible pairs, triplets, quads or even higher order multiplets were discussed in respect to Scatchard's mixing parameter values.

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

B-01-S**INSIGHTS FROM NUMERICALLY EXACT APPROACHES FOR THE CALCULATION OF THE ROVIBRATIONAL ENERGY STRUCTURE OF TRI- AND TETRATOMIC MOLECULES**M. Mladenović*MSME, Univ Gustave Eiffel, CNRS UMR 8208, Univ Paris Est Créteil, F-77454 Marne-la-Vallée, France (mirjana.mladenovic@univ-eiffel.fr)*

Numerically exact rotation-vibration solutions to the molecular Schrödinger equation for tri- and tetratomic molecules are applied. As a first example, the torsional structure of HOCO is analyzed using several adiabatic projection techniques. The torsional structure is found to exhibit two limiting cases associated with oscillator and rotor spectral patterns. Combining full-dimensional rovibrational calculations for N_2H^+ with the available experimental values for B_0 , the r_0 and r_e structures of the ion are additionally determined and analyzed.

B-02-S**STUDY OF NONCOVALENT INTERACTIONS USING CRYSTAL STRUCTURE DATA AND QUANTUM CHEMICAL CALCULATIONS**

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The analysis of the crystal structures in the CSD was used to recognize and characterize new types of noncovalent interactions. It was also used to study already known noncovalent interactions. Based on the data from the CSD we can determine existence of the interactions, frequency of the interactions, and preferred geometries of the interactions in the crystal structures [1,2].

The quantum chemical calculations were performed to evaluate the energies of the interactions. For the preferred geometries in the crystal structures we can calculate the interaction energies. By calculating potential energy surfaces for the interactions, we can determine the most stable geometries, as well as stability of various geometries [1,2].

Using this methodology our group recognized stacking interactions of planar metal-chelate rings; stacking interactions with organic aromatic rings, and stacking interactions between two chelate rings. The calculated energies showed that the stacking of metal-chelate rings is stronger than stacking between two benzene molecules. Studies of interactions of coordinated ligands indicate stronger noncovalent interactions than interactions of noncoordinated molecules [2].

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B-03-O**FORMATION OF THE METHANE HALIDES FLUID-LIKE LAYERS AT AMBIENT CONDITIONS**

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The work presents the IR-study of fluid-like methane halides (methyl iodide, carbon tetrachloride, chloroform, and methane dichloride) layers formation in the near-surface area at ambient conditions. It was shown that at vapors compression-expansion procedure in variable-thickness spectral cell, the phase state of matter, exhibiting both gas and liquid spectral properties appears. The reversible and continuous transition of gas-like and liquid-like shapes, not depending on thermodynamic characteristics of studied substances, was revealed.

B-04-O**STRUCTURAL TRANSFORMATIONS OF DICHLORO-ALKANES AT THE LIQUID-TO-GAS TRANSITION**

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The work discusses the data obtained by IR study referring to the dual gas-liquid properties of thin layers forming in the cell near-surface (optical windows) area for dichloromethane, 1,2-dichloroethane and 1,2-dichloropropane. These layers represent the combination of gas-like and liquid-like states, which can be considered as the intermediate stage of the phase transition from gas to liquid. It was shown that the molecular interactions in dual gas-liquid systems of chloroalkanes are changing due to the restructuring of Cl...H hydrogen bonding.

B-05-P**A THEORETICAL CALCULATION OF THE RAMAN SPECTRUM OF INDIGO CARMINE**J. Senćanski¹, J. Maksimović² and M. Pagnacco³

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This paper presents the B97D functional added to the Hamiltonian in order to calculate Raman spectrum of indigo carmine. The experimental spectrum of the compound was recorded from indigo carmine, a commercial dye sold for use in food processing when used in a mixture with D-glucose. The Raman spectrum was calculated using the B97D/cc-pVTZ level of theory. The results obtained show lower deviation from 1000 cm⁻¹ to 2000 cm⁻¹ for the main bands compared with the data found in the literature.

B-06-P**LIBS HYDROGEN DETECTION:
TEA CO₂ LASER - POLYMETHYL METHACRYLATE INTERACTION**M. Trtica¹, M. Kuzmanovic², J. Savovic¹ and D. Rankovic²

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Laser-Induced Breakdown Spectroscopy (LIBS) was applied to detect hydrogen in solid polymer - polymethyl methacrylate (PMMA). A pulsed Transversely Atmospheric Excited (TEA) CO₂ laser was used as the excitation source. Using a low laser intensity of ~58 MW/cm² and fluence of ~16.5 J/cm², the plasma above the PMMA was studied in a vacuum ambience (0.01 mbar). Under the applied experimental conditions, the plasma could be induced only in the presence of a metal sub-target, after a cavity in a PMMA was created by multipulse laser ablation. The spectrum of the plasma generated on a PMMA-metal sub-target system was dominated by the emission of intensive hydrogen, carbon, and oxygen atomic lines and molecular bands of C₂ and CN. The characteristics of laser-induced plasma were analyzed by evaluating the plasma parameters, such as the electron number density and temperature.

B-07-P**LASER-INDUCED BREAKDOWN SPECTROSCOPY STUDY OF ARCHEOLOGICAL GLASS SAMPLES**

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Two unclassified glass samples of medieval origin found in Belgrade were examined by the laser-induced plasma spectroscopy (LIBS) technique. Measurements were performed with a LIBS system based on a compact TEA CO₂ laser with low pulse energy ($E < 170$ mJ). The threshold energy required to induce plasma on a glass sample was 80 mJ per pulse. Depending on the sample, spectral lines of Si, Al, Ca, Fe, Ti, Mg, Mn, Sr, Cu, K, Ba, Na, and Ni were detected. Detection limits (LODs) were also estimated for several elements: Ni (18 ppm), Cu (2.5 ppm), Ti (25 ppm), Mn (32 ppm), and K (205 ppm). The plasma diagnostics was performed to determine plasma temperature and electron concentration. The excitation temperature of 8700 K was evaluated using a Boltzmann plot, constructed from the measured relative integral intensities of iron spectral lines. The electron number density, determined using the intensity ratio of Ti ionic and atomic lines, was $2 \cdot 10^{17}$ cm⁻³.

B-08-P**OPTICAL SPECTROSCOPY OF PLASMA INDUCED BY IRRADIATION OF ANIMAL BONE WITH TEA CO₂ LASER**

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The application of laser-induced breakdown spectroscopy (LIBS) for the elemental analysis of pig shoulder bone samples is reported. Measurements were performed using a compact laboratory-made TEA CO₂ laser with low pulse energy. The recorded spectra consisted of well-defined lines of atoms and single charged ions of Ca, Mg, P, and other constituent elements, with a good signal-to-noise ratio suitable for spectrochemical analysis. Based on the ICP quantitative analysis of the bone sample, the limits of detection of LIBS analysis were estimated for Mg (16 ppm) and Na (940 ppm). Plasma parameters, temperature, and electron number density were determined by measuring Stark widths and relative intensities of the C and Mg ionic and atomic spectral lines.

B-09-P**CONFORMATIONAL AND SPECTROSCOPIC ANALYSES OF
2-(4-FLUOROPHENYL)-2-HYDROXYPROPANOIC ACID**

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The conformational and vibrational spectroscopic analyses of 2-(4-fluorophenyl)-2-hydroxypropanoic acid (FHPA) are represented in this research. Theoretical calculations were performed by density functional theory (DFT) with B3LYP method using 6-311++G(d,p) basis set. The FT-IR and Raman spectra of FHPA were recorded and analyzed. The comparison between the experimental and calculated spectra showed good agreement. Molecular electrostatic potential map (MEP) of the compound was calculated to predict chemical reactivity of the title molecule.

B-10-P**SPECTROSCOPIC AND COMPUTATIONAL STUDY OF NOVEL
DIHYDROPYRIMIDINE AZO PYRIDONE DYE**Ž. Vitnik¹, J. Tadić², D. Mijin³ and V. Vitnik¹

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Structural, vibrational, electronic, NMR and reactivity properties of ethyl 4-(4-((5-cyano-2-hydroxy-4-methyl-6-oxo-1-propyl-1,6-dihydropyridine-3-yl)diazenyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (PPD) were investigated by using density functional theory (DFT). Theoretical calculations were performed with B3LYP/6-311++G(d,p) method. The calculated data correlated well with the experimental ones. HOMO-LUMO energy gap for the title molecule confirmed the high reactivity of dye. The obtained results verified the hydrazone form as more stable one. In addition, molecular electrostatic potential (MEP) map of the dye was used to test its activity.

B-11-P**EXPERIMENTAL AND THEORETICAL UV-VIS SPECTRAL STUDY OF SOME ARYLAZO PYRIDONE DYES IN AMIDE SOLVENTS**J. Lađarević¹, Ž. Vitnik², V. Vitnik², B. Božić³ and D. Mijin¹¹ Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia² Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia. (vesnak@chem.bg.ac.rs)³ Institute of Physiology and Biochemistry "Ivan Đaja", Faculty of Biology, University of Belgrade, Studentski trg 16, Belgrade, Serbia

Spectral properties of ten 5-(substituted phenylazo)-3-cyano-1-ethyl-6-hydroxy-4-methyl-2-pyridones were investigated in formamide and *N,N*-dimethylformamide (DMF) by combining experimental study and density functional theory (DFT). In these two solvents, equilibrium between hydrazone and anionic forms is confirmed both experimentally and theoretically. Relative position of the absorption maxima of hydrazone and anion forms is highly affected by the substitution pattern in the phenyl ring. Theoretical absorption energies showed good agreement with experimental data.

B-12-P**CRYSTALLOGRAPHIC AND DFT STRUCTURAL ANALYSIS OF OCTOPAMINE-COUMARIN DERIVATIVE**D. Dimić¹, E. Avdović², D. Sretenović³, Ž. Milanović², G. Kaluđerović⁴ and J. Dimitrić-Marković¹¹ University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11000 Belgrade, Republic of Serbia. (ddimic@ffh.bg.ac.rs)² Institute of Information Technologies, Department of Science, University of Kragujevac, Jovana Cvijića bb, 3400 Kragujevac, Serbia.³ Lehrstuhl für Molekulare Physikalische Chemie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D 40225 Düsseldorf, Germany.⁴ Department of Engineering and Natural Sciences, University of Applied Sciences Merseburg, Eberhard-Leibnitz-Straße 2, DE-06217 Merseburg, Germany

Octopamine is a norepinephrine analog in invertebrates and acts as a neurotransmitter. The crystal structure of a novel octopamine-coumarin derivative is described in this contribution. The density functional theory optimization of a structure by several common functionals (APFD, B3LYP-D3BJ, M05-2X, and M06-2X) was performed. Based on the bond lengths and angles, B3LYP-D3BJ proved to be the most reliable functional with the lowest values of mean absolute error. The experimental and theoretical UV-Vis transition wavelengths are also discussed.

B-13-P**DFT OPTIMIZATION AND FUKUI ANALYSIS OF SELECTED 1,4-BENZODIAZEPIN-2-ONE DRUGS**

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1,4-Benzodiazepin-2-ones are an important class of drugs with a variety of structural modifications. Five of them (nordiazepam, diazepam, oxazepam, temazepam, and nitrazepam) were optimized at the M06-2X/6-311++(d,p) level of theory based on the crystallographic structure. After the comparison, quantified by the correlation coefficient and mean average error, these structures underwent the Natural Bond Orbital (NBO) analysis and the Condensed Fukui functions (CFFs) were calculated. The most reactive positions for electrophilic, nucleophilic, and radical attack were determined.

B-14-P**THE NATURE OF STACKING INTERACTIONS OF THE RESONANCE-ASSISTED HYDROGEN-BRIDGED RINGS**

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The Symmetry Adapted Perturbation Theory (SAPT) energy decomposition analysis is applied for studying the nature of stacking interaction occurring in homodimers of resonance-assisted hydrogen-bridged (RAHB) rings and heterodimers of RAHB and benzene rings. The contribution of various energy terms is dependent on the composition of a RAHB ring and can be rationalized based on electrostatic potential maps.

C - Kinetics, Catalysis

C-01-S**ROLE OF MECHANOCHEMISTRY IN ECO-FRIENDLY AND SUSTAINABLE PREPARATION AND RECYCLING OF CATALYSTS**

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Ensuring a secure, reliable and unhindered supply of raw materials is crucial for the competitiveness and growth of the European Union (EU) economy. The EU is taking actions to secure the access of all raw materials, but some of them are defined as ‘critical’. Difficulties in the access to critical raw materials (CRMs) are expected to depress industrial sectors vital to European Union. The current conditions of material supply and their evolution in EU and international markets strongly affect the present-day list of CRMs. The current Fourth list of CRMs was published in 2020 and covers a larger number of materials. The sustainable solution of the CRM problem is design of advanced CRM-free or low content materials, but also the optimal use, enhanced recycling and sustainable mining. In this context, the European Commission set up a number of initiatives to promote innovative solutions and accelerate the innovations in the field of raw materials. A lot of efforts are concentrated on the substitution of CRMs together with preservation and improvement of the advanced properties of the respective materials. However the more realistic option relates to optimisation of CRM life cycle covering extraction and processing of the raw materials, manufacturing, distribution, use, recycling, and final disposal, as well as the environmental impact of a product through its life cycle.

Currently preparation of heterogeneous catalysts with advanced properties is strongly related to the use of one or more CRM such as Cr, rare earths, platinum group metals, etc. Criticality assessment of some raw materials in regard of catalysts preparation will be presented.

Mechanochemical treatment can be successfully used as a method for CRM recovery and recycling. On the other hand, the role of Mechanochemistry in synthesis and/or activation of CRM-free catalysts is a large and growing field of research and innovations. The research activities in this fast-moving area are focused on the development of new concepts for design and synthesis of non-CRM catalysts with the same or better activity and selectivity compared to the current ones. Improvement of full material life-cycle of obtained non-CRM catalysts together with better recycling, reuse and repair of CRM-based catalysts are open areas for new ideas, scientific and innovative projects.

C-02-S**ARTIFICIAL SECONDARY STRUCTURES IN THE DESIGN OF NEW CATALYSTS AND NEW MATERIALS**S. I. Kirin

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In this conference paper, an author's review in the field of bioinorganic chemistry, stereochemistry, homogeneous catalysis and medicinal inorganic chemistry is presented, with particular emphasis on physical chemistry aspects. Within this work, bioconjugates of amino acid containing phosphine or nitrogen ligands were utilized for metal coordination. The metal complexes were extensively characterized by a number of instrumental spectroscopic or crystallographic techniques and by DFT calculations. The metal complexes were used as catalysts in the selective preparation of intermediates in the synthesis of active pharmaceutical ingredients. Special attention was paid to the formation of specific supramolecular artificial secondary structures formed by the amino acid moieties that control the stereochemical outcome of the catalytic reactions. In addition, the metal complexes served as building blocks for supramolecular architectures as well as potent anticancer agents.

C-03-S**VISIBLE LIGHT PROMOTED PHOTOREDOX CATALYSIS IN MICROFLOW SYSTEMS**Bojan P. Bondžić

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Lately, the application of microfluidic devices has been a very promising strategy in organic chemistry, and one of the research fields in which microfluidics have shown great potential is visible light photochemistry. There are several advantages when conducting transformations in flow compared to the batch reactions, in particular: a more predictable reaction scale-up, decreased safety hazards, improved reproducibility and yields, shorter residence time, higher reaction selectivity and product purity and lower catalyst loading. In addition, for photochemical transformations, the high surface-area-to-volume ratios typical of flow reactors allow for improved light efficiency. Light penetration in batch reactors is limited by decreasing light transmission over distance in a liquid medium.

Having all these advantages in mind, it comes as no surprise that visible light promoted photoredox chemistry in flow has been applied in functionalizations biologically active organic molecules.

A merger of organocatalysis and visible light photoredox catalysis performed in flow allowed access to a wide range of functionalized N-aryl-substituted tetrahydroisoquinolines (THIQs) in a formal C–H oxidation/Mannich reaction. Strecker type functionalization and copper-catalyzed

alkynylation of several *N*-aryl-substituted THIQs were also successfully performed in flow, giving valuable products with high efficiencies. Three types of microreactors i.e., PFA microtube flow reactor, PDMS polymeric microreactor and glass/silicon reactor were designed and applied in these model reactions. The application of custom-made porous polymeric type microreactors proved to be crucial regarding the C–H oxidation step and overall reaction performance.

C-04-S

METAL DUSTING AS A KEY ROUTE TO PRODUCE FUNCTIONALIZED CARBON NANOFIBERS

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The catalytic chemical vapor deposition (CCVD) method is frequently used to produce carbon nanomaterials, which are characterized by unique properties. Such materials are applied in various fields of science and technology, and their attractiveness grows year by year. Both the size and chemical, and phase composition of the catalysts are responsible for their activity and stability. In some cases, amorphous carbon being formed blocks the active sites and thus interrupts the CCVD process. On the other hand, the metal dusting process, known as a negative phenomenon causing the destruction of the industrial metal reactors, has started to be considered as a preparative route to obtain active and stable CCVD catalysts from bulk metal precursors. The present paper is aimed to demonstrate the current state of art in the claimed field of science.

C-05-S

PEROXO-Zr/Hf CONTAINING POLYOXOMETALATES: SYNTHESIS, STRUCTURE AND DETAILED RAMAN SPECTROSCOPIC STUDIES

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Polyoxometalates (POM) are discrete anionic metal-oxo clusters of early *d*-block metal addenda ions in high oxidation states (e.g. W^{VI} Mo^{VI}, V^V). POMs exhibit a large variety of shapes, sizes and

compositions with multiple associated physicochemical properties and potential applications in catalysis, biomedicine and material science. The substitution of addenda atoms by other d or f-block metals such as Zr or Hf can lead to novel compounds with unprecedented properties, and some peroxo-derivatives are also known. Here we report on the synthesis and structural characterization of four novel peroxo-Zr and Hf-containing polyanions of the Wells-Dawson type. The solution stability was investigated by multinuclear NMR and detailed Raman and IR spectroscopic studies were performed in the solid state. The catalytic activity of the novel POMs in the H₂O₂-based oxidation of organic substrates was also investigated.

C-06-S

CATALYTIC PROPERTIES OF CARBON NANOTUBES AND REDUCED GRAPHENE OXIDE IN ETHYLENE HYDROGENATION BY MOLECULAR HYDROGEN

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In the last years, several studies dedicated to the carbon nanomaterials such as multi-walled carbon nanotubes (CNT) and reduced graphene oxide (rGO) catalytic activity in the hydrogenation reactions have been reported. Particularly, for the first time, we showed that rGO and CNTs are active in the gas-phase hydrogenation reactions with molecular hydrogen.

The work is dedicated to the determination of the influence of the structure and functionality of CNT and rGO on the catalytic activity in the hydrogenation of ethylene by molecular hydrogen. The ethylene hydrogenation is a simple model gas-phase reaction that convenient to establish a dependence between the method of catalyst activation, the diameter of CNT, and the procedure of rGO preparation and their catalytic activity.

The catalytic activity of rGO strongly depends on its structural characteristics. An increase in the surface area and a decrease in the oxygen content enhance the catalytic activity of rGO. The defectiveness and oxygen content are crucial for the catalytic performance of rGO obtained either by thermal reduction of graphene oxide in hydrogen or by reduction of graphene oxide with hydrazine. This conclusion has significant implications for the potential applications of rGO as a hydrogenation catalyst.

Obtained results show that non-activated carbon nanomaterials do not exhibit catalytic activity. Increasing the temperature of activation from 100°C to 400°C increases the catalytic activity by three orders of magnitude. Further temperature increase leads to a decrease in catalytic activity. An increase in the CNT diameter significantly decreases the catalytic activity. The highest obtained activity for CNT is $6.2 \cdot 10^{-6} \text{ mol} \cdot \text{s}^{-1} \cdot \text{m}^{-2}$ which is higher compared to rGO.

Our results indicate the high stability of CNT and rGO compared to the typical hydrogenation catalysts in hydrogen-rich and ethylene-rich atmospheres. That offers new opportunities for the application of nanocarbon-based catalysts in the hydrogenation reaction at high temperatures. That is extremely important to replace catalysts operating under conditions where the metal-containing catalysts deactivate due to the formation of the carbonaceous deposits.

C-07-S**PREDICTING PARTICLE SIZE DISTRIBUTION IN NANOPARTICLE FORMATION BY STOCHASTIC AND DETERMINISTIC APPROACHES**R. Szabó and G. Lente

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A class of nucleation-growth type models for nanoparticle formation were investigated by deterministic and stochastic kinetic methods. Four different kernel functions were used for characterizing the dependence of the reactivity of a nanoparticle on its size in the growth reaction. The final distribution of nanoparticles formed were determined as a function of the ratio of the rate constants characterizing nucleation and particle growth. It was found that the final size distributions predicted by the stochastic and deterministic approaches for the same model agree very well. Furthermore, it was also shown that the average size of nanoparticles formed can be given as a function of the rate constant ratio with a simple power expression, where the value of the exponent depends on the identity of the kernel function used.

C-08-O**FREE RADICAL SCAVENGING POTENCY OF EQUOL**A. Amić¹, D. Milenković², J. M. Dimitrić Marković³ and Z. Marković²

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Kinetic analysis performed by using Transitivity Code indicates that phenolic hydrogens of physiologically active equol molecule are much more abstractable than C-ring hydrogens. Obtained results are opposite to very recently published statements that aliphatic C–H bonds of natural compounds may play significant role in antioxidant action. Unequivocally, phenolic O–H bonds are responsible for antiradical activity of equol. The contribution of equol's C-ring hydrogens to free radical scavenging is negligible.

C-09-O**APPLICATION OF QUANTUM CHEMICAL CALCULATION IN DEFINING PEAKS IN UV-VIS SPECTRA OF OXIDATIVE TARTRAZINE DEGRADATION**

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Degradation of tartrazine in presence of cobalt activated Oxone[®] (potassium peroxydisulfate) was investigated. Aluminium pillared clay acted as a support for catalytically active Co²⁺. Oxone[®] was a precursor of SO₄^{•-} radical anions. Along with decolorization of tartrazine solution, the degradation of tartrazine and formation of oxidation products was monitored using UV-Vis spectroscopy. Quantum chemical calculations were performed in order to predict UV-Vis spectra. Different models were tested and the results of calculation have shown that the combination of TPSS-D3 method and aug-cc-pVDZ basis set is quite satisfactory level of theory. The experimentally obtained peaks that arose during degradation were identified using this method.

C-10-O**KINETICS OF THE REDUCTION OF DICYANOBIS(2,2'-BIPYRIDYL) IRON(III) BY IODIDE IN AQUEOUS MEDIUM**

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The redox reaction between dicyanobis(2,2'-bipyridyl)iron(III) and iodide may have potential application in dye-sensitized solar cells. In this study, kinetics of the reduction of dicyanobis(2,2'-bipyridyl)iron(III) was studied in aqueous medium. Iodide was used as a reducing agent at 60 mM ionic strength and a temperature of 293 ± 0.5 K. The reaction was of zero and fractional (0.5) order in the oxidant and reductant, respectively. The reaction was in general fractional (0.5) order. With increasing acidity in the reaction mixture, the measured zero order rate constant decreased, but was unaffected by increasing ionic strength. The thermodynamic parameters of activation were also computed for the redox process.

C-11-P

MODELING OF THE LINSEED OIL EPOXIDATION: THE USE OF DIFFERENT EXPRESSIONS FOR THE REACTION RATE OF THE PERACETIC ACID FORMATION

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The published pseudohomogeneous model for the vegetable oil epoxidation with *in situ* formed peracetic acid in the presence of the ion exchange resin as a catalyst was modified considering, besides the heterogeneously catalyzed, previously neglected homogeneously catalyzed peracetic acid formation. Comparison of the original and two proposed models shows that introduced modification improves the modeling of the epoxidation process.

C-12-P

EFFICACY OF ZIRCONIA BASED NANOPOWDERS IN REMOVAL OF PHARMACEUTICALS USING SOLAR IRRADIATION

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Photocatalytic/adsorption efficacy of pure ZrO₂ and ZrO₂ powders with incorporated Si⁴⁺ ions was obtained following kinetics of degradation reaction and adsorption/desorption of some pharmaceuticals under solar irradiation. All selected pharmaceuticals have been found in surface waters in Serbia as organic micropollutants with ability to impact water quality, ecosystems and human health. Removal efficacy was followed using UFLC technique. All used zirconia based nanopowders can be used for removal of selected pharmaceutical.

C-13-P**ZIRCONIA BASED PHOTOCATALYSTS IN DEGRADATION OF SELECTED HERBICIDES**

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Hydrothermally synthesized zirconia nanopowders: pure and doped with Si⁴⁺ ions were spectroscopically characterized and used as photocatalysts for degradation of herbicides sulcotrione and fluroxypyr. Zirconia is wide band gap ceramic ($E_g \sim 5$ eV) however, synthesized nanopowders showed unexpected, modest absorbance in visible light range. That fact inspired photocatalytical degradation of herbicides with wide utilization, using solar irradiation (SI) in laboratory conditions. In the scope of this study, degradation of herbicides was only slightly achieved (irradiation time 2h).

C-14-P**COBALT SUPPORTED CHITOSAN-DERIVED CARBON-SMECTITE COMPOSITE FOR CATALYTIC ACTIVATION OF PEROXYMONOSULFATE IN WATER**

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In this work cobalt supported on chitosan-derived carbon-smectite composite catalyst was synthesized using impregnation-carbonization method (Co/cCh-S). The carbonization temperature was 400 °C. The obtained catalyst was tested as peroxymonosulfate (in form of Oxone[®]) activator for the food dye tartrazine degradation. The textural properties were obtained using low temperature N₂ physisorption. The calculated textural parameters of the Co/cCh-S catalyst were compared with properties of the carbonized chitosane-smectite composite (cCh-S). The catalytic tests confirmed that neither Oxone[®] without catalyst nor cCh-S were unable to activate Oxone[®]. The catalyst Co/cCh-S was found to be effective for tartrazine degradation in presence of Oxone[®].

C-15-P**HYDROGEN PRODUCTION FROM GLYCEROL PHOTO-REFORMING OVER PT/N-DOPED TITANATE PHOTOCATALYSTS**

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Conversion of sunlight energy via photocatalytic water splitting and photo-reforming of renewable biomass organic derivatives has been increasingly utilized for hydrogen production. Photocatalytic processes have been used due to their sustainability, environmental-safety, and effectiveness. Pt/N-doped titanate photocatalysts were synthesized via alkaline hydrothermal treatment, followed by $\text{Na}^+/\text{NH}_4^+$ ion exchange, impregnation and gaseous reduction. The activities of the photocatalysts were tested for hydrogen production via photocatalytic reforming of glycerol under simulated solar irradiation. The improved hydrogen production from photo-reforming of glycerol was attributed to the anatase active phase and surface area which enhanced the adsorption of glycerol onto the surface of catalysts; metallic Pt suppress the electron/hole recombination by trapping the photo-generated electrons; reduced band gap by incorporation of N into lattice of TiO_2 .

C-16-P**PHOTODEGRADATION OF DYES USING G-C₃N₄/TiO₂-BASED NANOCOMPOSITE**

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Titanium dioxide is one of the most studied photocatalysts, using only the UV part of the light spectrum. There are various methods for improving the photocatalytic activity of TiO_2 , such as activating TiO_2 in the visible part of the light spectrum. Titanium and carbon nitride-based hybrid photocatalyst was successfully synthesized by hydrothermal method followed by thermal treatment of a physical mixture of melamine and titania nanowires. The prepared nanocomposite was used to remove model pollutants - Methylene Blue (MB) and Acid Orange 10 (AO10) from its water solutions. Besides investigating the influences of cationic and anionic dyes on adsorption and photodegradation using solar light spectrum, varying the concentration of MB was examined under the visible light spectrum.

C-17-P**SURFACE ELECTRONIC STATE AT CeO₂-MODIFIED DIATOMITE AND SILICA GEL SUPPORTS**

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The effect of cerium oxide modification of two different SiO₂ supports diatomite (macroporous natural origin material) and commercial silica gel (mesoporous industrial material) was examined. UV-vis diffuse reflectance and X-ray photoelectron spectroscopy measurements were used for estimation of the surface electronic state at both modified SiO₂ supports combine with data of X-ray diffraction, N₂ physisorption technique and electron paramagnetic resonance. Ce³⁺ ions were found in the supported CeO₂ structure over both SiO₂ supports after calcination at 400 °C. The CeO₂ modification reflects on the texture properties and surface electronic state by stronger Ce–O–Si bond in the case of modified CeO₂-silica gel support.

C-18-P**INFLUENCE OF THE SURFACE SPECIES ON THE CATALYTIC PERFORMANCE OF Co-Pd CATALYSTS IN CO HYDROGENATION. PART 1. ROLE OF TITANIA SUPPORT**

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Activity and selectivity of (10%Co+0.5%Pd)/TiO₂ system in CO hydro-genation were studied in dependence of pretreatment mode, reduction and reaction temperature. It aimed to evaluate the information about influence of surface species and sites on catalytic performance. Samples were preliminary treated in oxidative, reductive, or inert gas flow and studied by chemisorption of H₂ and CO, TPR, XPS, EPR, *in situ* DRIFTS and catalytic measurements. Dependence on the mode of pretreatment and reduction temperature on the catalyst activity in CO conversion and selectivity to CH₄ were found. The reductive pretreatment resulted in an active sample characterized by bridged CO species on metal sites with weakened C-O bond that facilitated cleavage at lower temperatures and more bidentate carbonate species on average strength sites. The selective catalyst was prepared by pretreatment in air and revealed predomination of formate and monodentate carbonate species on strong adsorption sites of TiO₂.

C-19-P**INFLUENCE OF RESIDENCE TIME ON THE DECOMPOSITION RATE OF OLEYLAMINE**

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Film forming amines (FFA) are organic feedwater additives used in the power industry for several decades. Even though, the utilization of FFA in power plants is highly dependent on their thermal stability in the high temperature water/steam environment, the scientific data are scarce. Oleylamine (OLA) is known to be a film forming amine commonly applied in power industry as a feedwater additive for the corrosion protection of the steam generators. The decomposition rate of OLA was studied at the temperatures up to 220 °C. For this purpose, the novel experimental high-temperature high-pressure stainless steel reactor was employed. The reactor was operational up to 300 °C/200 bar. For determination of the OLA concentration, the Bengal Rose method was used. In this paper, the effect of the residence time on the decomposition rate was presented. The obtained results demonstrated a high decomposition rate of OLA.

C-20-P**INFLUENCE OF THE SURFACE SPECIES ON THE CATALYTIC PERFORMANCE OF Co-Pd CATALYSTS IN CO HYDROGENATION. PART 2. ROLE OF ALUMINA AND SILICA SUPPORT**

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Activity in CO conversion and selectivity to CH₄ of bimetallic catalysts Co-Pd/Al₂O₃ and Co-Pd/SiO₂ were studied in dependence of support, pretreatment mode, reduction and reaction temperature. Research was focused on the effect of surface sites and species on catalytic action. Samples were pretreated in air, H₂, or Ar and studied by H₂ and CO chemisorption, TPR, catalytic measurements, XPS, and EPR. The pretreatment in air resulted in formation of active samples with more pure Co and Pd particles and bridged CO species with weakened C-O bond that facilitated activation at lower temperatures. However, the high quota of unreduced metal and hydroxyl groups on the support with average strength sites for carbonate species adsorption facilitated WGS. Selective catalysts were obtained by pretreatment in H₂ or Ar and were characterized by low

level of unreduced metal, more bimetallic particles, more sites for strong adsorption of carbonate species on Al₂O₃.

C-21-P**APPLICATION OF EPR SPECTROSCOPY FOR SILVER-BASED CATALYSTS CHARACTERIZATION**

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EPR spectra of oxidized 15Ag15CeO₂/SiO₂ registered in the temperature range 123-323 K show two overlapping signals – a broad line due to silver clusters and a narrow one due to the presence of Ag⁰ species. In view of the obtained EPR results it can suppose that Ag clusters in oxidized 15Ag15CeO₂/SiO₂ catalyst are destroyed and Ag⁺ and Ag⁰ are formed during catalytic reaction. EPR spectra of H₂-treated samples show that there is no EPR spectrum of silver clusters and only Ag⁰ were detected. After the catalytic reaction, the shape and parameters of EPR spectrum of reduced 15Ag15CeO₂/SiO₂ catalyst is not changed.

C-22-P**PHOTOCATALYTIC AND ELECTROCATALYTIC OXIDATION OF 2,4,6-TRICHLOROPHENOL ON IRON-DOPED NANOZIRCONIA CERAMIC**

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Photocatalytic and electrocatalytic oxidation of 2,4,6-trichlorophenol (TCP) was investigated on pure and iron-doped zirconia matrix synthesized by solvothermal method from organometallic precursors. The doping of zirconia with Fe³⁺ ions had beneficial effect on its photocatalytic performance in degradation of TCP. Electrocatalytic investigation showed that TCP oxidation pathway depended on iron ions content in zirconia matrix.

C-23-P**COBALT-DOPED ALUMINA CATALYSTS IN CATALYTIC OXIDATION OF TARTRAZINE INDUCED BY OXONE®**

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In this work cobalt-doped alumina catalysts were synthesized using the sol-gel method. The calcination temperatures were 500 °C, 1000 °C and 1100 °C and the catalysts were denoted as CoA-500, CoA-1000 and CoA-110, respectively. The obtained catalysts were tested as Oxone® activators for the degradation of tartrazine azo-dye. The influence of the mass of catalyst and the reaction temperature was investigated. The catalyst mass and temperature increase were beneficial for the dye degradation rate. All three catalysts were found to be effective for tartrazine degradation in the presence of Oxone®.

C-24-P**KINETIC AND THERMODYNAMIC STUDY OF THE OXIDATIVE CATALYTIC DEGRADATION OF ACID ORANGE 10 IN THE PRESENCE OF OXONE® AND COBALT BASED CATALYST**

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Catalytic degradation of Acid Orange 10 in the presence of Oxone® activated by Co-impregnated acid activated montmorillonite as catalyst was investigated. The catalytic experiments were performed at different temperatures in range from 303 to 333 K in order to determine kinetics parameters. The kinetics data followed the first-order kinetics model. The activation energy of the investigated degradation process was calculated according to the Arrhenius equation.

C-25-P**CORROSION PROTECTION OF STAINLESS STEEL BY ZrO₂ AND ZrO₂-TiO₂ SOL-GEL COATINGS**

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Sol gel ZrO₂ and ZrO₂-TiO₂ composite coatings were deposited on stainless steel substrates and treated at 300 and 500°C, respectively. X-ray diffraction analyses (XRD) have proved the cubic ZrO₂ phase in zirconia coatings, while the composites coatings possess amorphous structure. The AFM analyses revealed typical island structure. It was registered that Zr-Ti composites are amorphous after treatment even at 500°C. The corrosion and electrochemical behavior of the samples was evaluated by potentiodynamic polarisation (PDP) under DC conditions. The coatings treated at 500°C exhibit higher corrosion resistance than the other sample types. This could be explained by the amorphous structure of the composites, which slows down the ionic and electron conductivity and the stabilizing role of ZrO₂ on the mechanical properties of titania.

C-26-P**PREFERENTIAL CO OXIDATION IN HYDROGEN-RICH GASES OVER Ag CATALYSTS SUPPORTED ON DIFFERENT SUPPORTS**

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Silver samples were prepared by impregnation of different supports (SiO₂, Al₂O₃, ZSM-5 (Si:Al=100)) with aqueous solution of AgNO₃. The catalysts were characterized by X-ray diffraction, X-ray photoelectron spectroscopy, temperature-programmed reduction and high-resolution SEM. It is established that the support has an important effect on the Ag phase composition, oxidation state, particle size distribution, and interaction between silver and the support. Samples supported on SiO₂ show better performance in the preferential CO oxidation in hydrogen rich gases.

*D - Nonlinear Dynamics,
Oscillatory Reactions,
Chaos*

D-01-S**VARIOUS DYNAMICAL STATES IN THE BRAY LIEBHASKSKY OSCILLATORY REACTION- FROM PERIODICITY TO INTERMITTENT CHAOS**A. Ivanović-Šašić¹, S. Maćešić², Ž. Čupić¹ and Lj. Kolar-Anić^{1,2}¹*University of Belgrade, Institute of Chemistry, Technology and Metallurgy, National Institute of Republic of Serbia, Belgrade, 11000 Serbia (ana.ivanovic@nanosys.ihm.bg.ac.rs)*²*University of Belgrade, Faculty of Physical Chemistry, Belgrade, 11000 Serbia*

The Bray-Liebhafsky (BL) is one of the most analyzed oscillatory reaction both experimentally and numerically. Most of the experimentally obtained dynamical states of this reaction realized in a continuously fed well stirred tank reactor (CSTR) are successfully simulated. Beside others, numerous structured chaotic dynamical states were obtained between each two periodic states in the period doubling rout to chaos with respect to specific flow rate as the control parameter. It was an universal scenario throughout the whole mixed-mode region, as well as throughout other mixed-mode regions obtained under different initial conditions. However, the intermittent oscillations consistent of chaotic mixture of large-amplitude relaxation oscillations, grouped in bursts and small-amplitude sinusoidal ones or even quiescent parts between them known as gaps were also generated experimentally in the Bray–Liebhafsky reaction by varying different parameters such as temperature, flow rate or reactant concentrations under CSTR conditions. Nevertheless, it will be shown here that intermittent oscillations can be simulated by already published model of the BL reaction network.

D-02-S**DYNAMICS OF HYDROXIDE-ION-DRIVEN AUTOCATALYTIC REACTION NETWORKS**

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In biochemistry, hydrogen bonding is an essential structure forming factor, therefore function and activity of enzymes strongly depend on the pH of the medium. Acid-base equilibria are needed to maintain physiological pH to attenuate fluctuations in hydrogen ion concentration. Redox reactions generally change the pH and because their rate depends on it, they often autocatalytic with respect to hydrogen ion. The positive feedback can provide the fundamental nonlinearity necessary in controlling far-from-equilibrium systems. However, an autocatalytic reaction under the mild conditions of organic molecules must interact with the acid-base equilibria present. Imines, for example, hydrolyze with their rate depending on the pH of the solution. For those, where hydrolysis rate is negligible in acidic medium, we show that their clock reaction, both substrate-depleting and autocatalysis driven, is a result of the delicate interplay between the autocatalytic hydroxide ion production and the acid-base equilibria of the components. With the addition of a reaction removing hydroxide ion we can, in principle, obtain oscillatory dynamics in an open system.

D-03-S**A BZ ASSEMBLAGE WORKING FOR A DAY**

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Our work is focused on the experimental observation of Bielousov-Zhabotinsky reaction oscillations in ferroin loaded Dowex 50w beads in a batch reactor open to the atmosphere. We investigated the conditions for the maximum oscillation lifetime and the change of wave regimes as the answer to the applied potential. The catalyst-free solution in the batch reactor is a mixture of concentrated sulphuric acid, NaBrO₃, and different ratios of malonic acid and 1,4- cyclohexanedione. We are using three types of cation Dowex 50w beads, namely type x2, x8, which differ by their level of crosslinking and cation exchange capacity. Their mesh size is 16-50 and 50-100. We investigate the influence of such parameters as the distance between a bead and the electrode and the value of electrode potential on the oscillations. Moreover, we study the character of oscillations in the function of the number of adjacent beads and the layout of the beads.

The reduction of formation of CO₂ bubbles has been achieved by choice of Dowex beads type, solution composition, and usage of acetone.

We report oscillations with stable amplitude and varying period and lifetime over 19 hours and oscillations with decreasing amplitude with a lifetime of 10 hours. The investigated media and beads type seem to be promising candidates for experimental realization of chemical computers based on interacting oscillators.

D-04-S**IMPACT OF D₂O ON SPONTANEOUS OSCILLATORY PEPTIDIZATION OF SELECTED α -AMINO ACIDS**

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Earlier, we have demonstrated spontaneous oscillatory chiral inversion and spontaneous oscillatory peptidization running with proteinogenic α -amino acids in the parallel. These processes might have been of certain importance in the prebiotic history of Earth, i.e., in the period of chemical evolution. In fact, spontaneous oscillatory peptidization can be regarded as a sequence of elementary steps which in certain sense simulate Life. On the other hand, it is a well recognized fact that heavy water (D₂O) considerably slows down life processes of all organisms and when dispensed in considerable amounts to organisms on a higher level of cellular organization (e.g., to mammals), it can exert even a lethal effect. As proteinogenic α -amino acids can be regarded as the smallest building blocks of all living

matter, now we are interested to find out, if D₂O can hamper spontaneous oscillatory peptidization of proteinogenic α -amino acids. In our study, we focused on three endogenous (L-Cys, L-Pro, L-Ala) and two exogenous (L-Met, L-Hyp) α -amino acids and we managed to demonstrate that D₂O strongly inhibits spontaneous oscillatory peptidization of all these compounds. It is noteworthy to add that out of five α -amino acids investigated so far, which can be divided into two groups of endogenous and exogenous species, two endogenous species (L-Cys and L-Pro) undergo spontaneous oscillatory peptidization following the circadian rhythm, whereas two exogenous ones (i.e., L-Met and L-Hyp) do not. The third endogenous species (L-Ala) first undergoes two initial oscillations which are damped (not periodic) and the oscillatory changes are on a scale of about 10 hours (as estimated with use of the Fourier Transform approach) and after that, the system reaches a steady state.

D-05-S

A METHODOLOGY FOR VERTICAL TRANSLATION BETWEEN MOLECULAR AND ORGANISMAL LEVEL IN BIOLOGICAL FEEDBACK LOOPS

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Feedback loops are among the primary network motifs in living organisms, ensuring survival via homeostatic control of key metabolites and physical properties. However, from a scientific perspective, their characterization is unsatisfactory since the usual modelling methodology is incompatible with the physiological and biochemical basis of metabolic networks. Therefore, any “vertical translation”, i.e. the study of the correspondence between molecular and organismal levels of causality, is difficult and in most cases impossible.

As a viable solution, we demonstrate an alternative modelling platform for biological feedback loops that is based on key biochemical principles, including mass action law, enzyme kinetics, binding of mediators to transporters and receptors, and basic pharmacological properties. Subsequently, we show how this framework can be used for translating from molecular to systems-level behaviour.

Basic elements of the proposed modelling platform include Michaelis-Menten kinetics defining nonlinear dependence of the output $y(t)$ on an input signal $x(t)$ with the Hill-Langmuir equation $y(t) = G * x(t)^n / (D + x(t)^n)$, non-competitive inhibition for linking stimulatory and inhibitory inputs with $y(t) = G + x_1(t) / ((D + x_1(t)) * (1 + x_2(t) / K_I))$ and processing structures for distribution and elimination.

Depending on the structure of the feedback loop, its equifinal (steady-state) behaviour can be solved in form of polynomials, with a quadratic equation for the simplest case with one feedback loop and a Hill exponent of 1, and higher-grade polynomials for additional feedback loops and/or integer Hill exponents > 1 . As a companion to the analytical solution, a flexible class library (CyberUnits) facilitates computer simulations for studying the transitional behaviour of the feedback loop.

Unlike other modelling strategies in biocybernetics and systems biology, this platform allows for straightforward translation from the statistical properties of single molecules on a “microscopic” level to the behaviour of the whole feedback loop on an organismal “macroscopic” level. An example is the Michaelis constant D , which is equivalent to $(k_{-1} + k_2) / k_1$, where k_1 , k_{-1} and k_2 denote the rate

constants for the association and dissociation of the enzyme-substrate or receptor-hormone complex, respectively. From the perspective of a single molecule the rate constants represent the probability (per unit time) that the corresponding reaction will happen in the subsequent time interval. Therefore $1/k$ represents the mean lifetime of the complex. Very similar considerations apply to the other described constants of the feedback loop.

In summary, this modelling technique renders the translation from a molecular level to a systems perspective possible. In addition to providing new insights into the physiology of biological feedback loops, it may be a valuable tool for multiple disciplines of biomedical research, including drug design, molecular genetics and investigations on the effects of endocrine disruptors.

D-06-S

NULLCLINES. A SIMPLE EXPLANATION OF COMPLICATED PHENOMENA

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To simply explain the sometimes-surprising results obtained with acidic solutions of hydrogen peroxide, iodate and iodine, we study the properties of the concentration space. The shape of the trajectories is determined by the slow manifold which can be reduced to a one-dimensional curve, the nullcline. In iodate-rich systems, it has the classic S-shape which explains the Bray-Liebafsky oscillations, their domain of existence and the effect of additions of different reagents. In low iodate systems, it can be more complicated and explains the unusual behavior of the iodine oxidation by hydrogen peroxide. The observed effects of oxygen are qualitatively explained by its effect on the nullcline.

D-07-S**THREE DECADES OF OSCILLATORY CARBONYLATION REACTIONS OF ALKYNES: PAST, PRESENT AND FUTURE**

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First reported in 1997, oscillatory carbonylation reactions of alkynes are still attracting our attention. Here, we summarize work thus far and share a vision of where these mesmerizing chemical oscillators may take us. We showcase a range of substrates, catalysts and solvents that successfully yield oscillations in redox potential, pH, turbidity and release reaction heat in a pulsatile manner. Moving towards prospective applications we look into transitioning this oscillatory carbonylation reaction from small molecule substrates and catalysts, to oscillatory reactions using polymeric substrates and catalysts, which are seen as the way forward in the formulation of oscillatory (pulsatile) materials.

D-08-S**REACTION NETWORK ANALYSIS OF CIRCADIAN AND ULTRADIAN RHYTHMS OF CYANOBACTERIA IN A PHOTOBIOREACTOR**Igor Schreiber*[†], František Muzika* and Jan Červený[†]**Department of Chemical Engineering, University of Chemistry and Technology, Prague, Czech Republic**[†]Department of Adaptive Biotechnologies, Global Change Research Institute, Academy of Science of the Czech Republic, Brno, Czech Republic*

Reaction network analysis assumes that stoichiometric equations are given for each reaction step together with power law rate expressions. On output, elementary subnetworks (known also as elementary modes or extreme currents) are identified and their capacity for displaying dynamical instabilities, such as bistability and oscillations, is evaluated by examining the associated Jacobian matrix. This analysis is qualitative and does not assume the rate values of coefficients and concentrations of chemical components. In the next step, the subnetworks are combined to form the entire network and its stability is deduced from the stability of the constituting subnetworks. In the final step, this combination principle is used in a quantitative manner for kinetic parameter estimation of the unknown/unspecified rate coefficients by applying linear optimization to a set of constraint equations balancing linearly combined subnetworks with the corresponding rate expressions. From mathematical point of view, this is a special case of convex optimization.

From the application point of view, the outlined theory is applied to experimentally measured activity of photosynthesizing diazotrophic cyanobacteria in a photobioreactor. In particular, we focus on biochemical processes giving rise to experimentally observed change from a steady state to oscillatory dynamics. The oscillations in cyanobacteria come from either a circadian clock synchronized with external light/dark cycle or from an internal ultradian cycle, which is active even in the absence of external environmental cues. For the former, we examine models of circadian clock

associated with a network involving the KaiABC proteins and their regeneration via a transcriptional network, for the latter, a compartmental model of carbon-nitrogen metabolism is analyzed.

For the metabolic model the set of unknown kinetic parameters is estimated via linear optimization so that the dynamics displayed by the model coincides with the experimentally observed emergence of oscillations.

D-09-S

ON THE INTERACTION OF EDTA WITH THE H₂O₂-NASCN-NAOH-CUSO₄ OSCILLATOR - FROM TRIVIAL ASSUMPTION TO A NEW KINETIC MECHANISM

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Oscillatory chemical reactions have been successfully studied for several decades. Recently, interest has been growing in coupled oscillators or single systems chemically perturbed by adding a substance that interacts with key intermediates of oscillatory systems. One of the most interesting systems of this type is the H₂O₂ - SCN⁻ - OH⁻ - Cu²⁺ oscillator discovered by Orbán [1] (which is often referred to as the Orbán-Epstein oscillator), and later studied in various research groups (cf. e.g. [2, 3, 4]), including our group (cf. e.g. [5, 6]).

In our recent extensive potentiometric and spectrophotometric studies of the effect of Cu²⁺ concentration on the dynamics of the Orbán-Epstein oscillator, modified by addition of EDTA, for a certain concentration range of [EDTA] < [CuSO₄], only transient damping of the oscillation amplitude was observed. Discovered in this way, non-trivial chemical interaction of EDTA with the oscillatory system made it possible to propose a new kinetic reaction mechanism of these phenomena, based on the perturbation of the oscillator feedback loops. The proposed chemical reaction scheme [7] has been illustrated by its numerical modeling, allowing for the estimation of the rate constants of individual reaction steps. Furthermore, the previously proposed [5] mechanism of differences in potentiometric responses of various inert electrodes was confirmed. In conclusion, the oscillatory H₂O₂ - SCN⁻ - OH⁻ - Cu²⁺ reaction has become a dynamic sensor of EDTA interactions with the components of the feedback loops.

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D-10-P

EXPERIMENTAL SETUP FOR CONTINUOUS MEASUREMENTS OF GASEOUS OXYGEN PRODUCTION IN BRAY-LIEBHAFSKY OSCILLATOR

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Experimental setup for tracing gas evolution in Bray-Liebhafsky (BL) oscillatory reaction was designed. It enables simultaneous and continuous recording of potential changes as well as relative gaseous pressure above BL reaction mixture. Since one serious problem in establishing reaction mechanism is limited number of techniques for monitoring reaction components, development of the cheap method for measuring evolved oxygen may be valuable.

D-11-P

DEVELOPMENT OF A SMART HYDROGEL OSCILLATOR

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The overall aim of this work is the synthesis and characterisation of hydrogels that have the ability to oscillate in volume to ultimately achieve an autonomous pulsed release system for drugs. To create a material capable of achieving this feat the incorporation of components that can produce oscillations in pH are required. Thorough testing of these components is required to ensure fulfilment of this role. The main components of this hydrogel include a polymeric catalyst and substrate that can work in tandem to produce a conformational response of a hydrogel system at specific intervals. Prior to assembling the hydrogels, the functionality of the catalyst and substrate require confirmation for yielding pH oscillations over longer periods of time (e.g. days).

D-12-P

CIRCADIAN RHYTHM FUNCTION COUPLING TO THE UPGRADED HYPOTHALAMIC-PITUITARY-ADRENAL (HPA) AXIS WITH INCORPORATED ARGININE VASOPRESSIN

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An upgraded model of the Hypothalamic-Pituitary-Adrenal (HPA) axis has been developed that advances our previously proposed low-dimensional HPA model by including the effects of arginine vasopressin (AVP) that is a key modulator of HPA axis function. The upgraded model allows us to emulate AVP effects on HPA axis dynamics individually and in synergy with the corticotropin-releasing hormone (CRH). In this work, we examine how coupling of the circadian function through summarised reaction steps describing CRH and AVP biosynthesis in the same neuronal cell group of the hypothalamic paraventricular nucleus (PVN) affects HPA axis dynamics. Results of numerical simulations show that coupling of the circadian function through both, CRH and AVP summarised biosynthesis reaction steps simultaneously, emulates best the HPA axis dynamics, in line with literature findings.

D-13-P

STOICHIOMETRIC NETWORK ANALYSIS OF THE MODEL OF OSCILLATORY CARBONYLATION OF PEGA IN OPEN REACTOR

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Subset of reactions of the model of palladium-catalysed oscillatory carbonylation of PEGA was analyzed. Stability analysis was then performed using stoichiometric network analysis (SNA). It was found that considered sub-model can simulate Andronov-Hopf and saddle-node bifurcations.

D-14-P

AUTOCATALYSIS OF HIO AND ASSOCIATED REACTION-DIFFUSION FRONTS IN THE MODEL OF BRAY-LIEBHAFSKY REACTION

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Analysis of the HIO autocatalytic production in the model of Bray-Liebhafsky reaction was carried out. 1D reaction-diffusion simulations were performed on the two subsets of reactions of the BL model responsible for functioning of the cycle where autocatalytic production of HIO occurs. Characteristics of these two reaction subsets and reaction-diffusion fronts emerging from them were analyzed.

D-15-P

QUANTUM ASPECTS AND IMPLICATIONS OF ELECTROCOALESCENCE PROCESS

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This is a brief presentation of multi-decennial work, at first as applied research and development (R&D), and later on as a fundamental research. In the pilot plant for uranium extraction from wet phosphoric acid the solution of entrainment problem was realized, that is breaking of double emulsions was explained, in some extent. Possible quantum aspects and implications, based on electrohydrodynamics principles and a theory or program of decoherence are discussed.

D-16-P

IMPACT OF D₂O ON PEPTIDIZATION OF L-ALANINE

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The investigation was carried out to collect experimental evidence on the effect of heavy water (D₂O) on spontaneous peptidization of proteinogenic α -amino acids upon an example of L-alanine (L-Ala). As analytical techniques, we used high-performance liquid chromatography with the diode array detection (HPLC-DAD), mass spectrometry (MS), and scanning electron microscopy (SEM). Growing proportions of D₂O in the reaction mixture result in decreasing yields of both, the soluble lower molecular weight peptides and the insoluble higher molecular weight peptides.

D-17-P

TANGENTIAL MODEL OF MICROTUBULES

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Microtubules (MTs) represent basic components of a cytoskeleton. The present work studies nonlinear dynamics of MTs assuming tangential oscillations of the dimers. We introduce a two-component model and show that the dynamics of MTs can be explained in terms of breather solitary waves.

D-18-P

MICRO-QUANTITATIVE ANALYSIS OF TYROSINE

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The biological importance of tyrosine interactions with iodine led us to investigate the possibilities of quantitative determination of tyrosine in the Bray-Liebhaufsky reaction using the pulse perturbation technique. For this purpose, a bifurcation diagram with respect to temperature was obtained, and the response of the Bray-Liebhaufsky system to tyrosine perturbations was examined. Tyrosine affects the temporal evolution of the system quantitatively in the micromolar range of concentrations. This finding suggests the possibility of using a Bray-Liebhaufsky matrix to quantify tyrosine.

E - Electrochemistry

E-01-O**ELECTROCHEMICAL DEPOSITION OF NEODYMIUM AND PRASEODYMIUM ON MOLYBDENUM FROM MOLTEN FLUORIDE**

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Neodymium and praseodymium were electrochemically co-deposited onto Mo cathode applying constant potential, from fluoride-based molten salts containing the corresponding rare earth oxides. According to the recorded voltammograms, it appears that in the investigated system, the electrodeposition of neodymium proceeds as a two-step reduction process: Nd(III)→Nd(II) and Nd(II)→Nd(0), whilst the praseodymium deposition proceeds as an one-step reduction process: Pr(III)→Pr(0). However, it was also recognized that at the same time a substantial amount of NdF₂ was formed as a result of the disproportionation reaction between the electrodeposited Nd metal and Nd(III) present in the electrolyte.

The deposit on the working electrode surface was recorded by optical microscopy and analyzed by X-ray diffraction (XRD). The analysis made upon the applying the potentiostatic deposition regime has shown Nd/Pr metals present on the molybdenum cathode.

E-02-P**MORPHOLOGY OF ALUMINIUM ELECTRODEPOSITED ON ALUMINIUM FROM AlCl₃+UREA SOLVATE IONIC LIQUID**

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The ionic liquid, made of urea and AlCl₃, known as deep eutectic solvent (DESs) has already shown to be low-cost electrolyte suitable for aluminum electrodeposition. By applying appropriate potentiostatic or galvanostatic electrolysis regime, aluminium is successfully electrodeposited from the deep eutectic solvent onto aluminium substrate at nearly room temperatures. Morphologies of the produced deposits were characterized by scanning electron microscopy (SEM) and chemical composition by energy-dispersive X-ray (EDX) analysis. The electrodeposited aluminium displayed different morphology depending on the deposition conditions applied.

E-03-P**IMPACT OF CURRENT DENSITY ON THE ELECTROCHEMICAL DEGRADATION OF PHENOL AT PbO₂-GNR ANODE**

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This paper presents the impact of current density on the degradation efficiency of phenol by electrochemical oxidation in the base media on a new hydrothermally synthesized PbO₂-GNR (lead dioxide – graphene nanoribbon) anode. The morphological characteristics of materials was obtained using field emission scanning electron microscopy (FESEM). The electrochemical oxidation were performed in galvanostatic mode applying current densities of 50 and 100 mA cm⁻² in 0.1 M Na₂SO₄. Experimental results have shown that the degradation efficiency increased with increasing applied current density and electrolysis time. After 60 minutes of the electrolysis the degradation efficiency of the phenol was 98.6 % and 49.4 % on current densities 100 and 50 mV cm⁻², respectively. The newly synthesized anode material PbO₂-GNR can be successfully used in the treatment of phenol-contaminated wastewater.

E-04-P**DEGRADATION OF RHODAMINE B DYE ON GRAPHITE ANODE: KINETIC AND ELECTROCHEMICAL BEHAVIOR**

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The aim of this study was to investigate the removal efficiency of Rhodamine B dye from NaCl aqueous solution by electrochemical oxidation on the graphite anode with a specific focus on the kinetics of the process. After 60 minutes of galvanostatic electrolysis on the applied current density of 25 mA cm⁻² removal efficiency of about 97.6% was obtained. The degradation of Rhodamine B fitted well with the first-order kinetics.

E-05-P**COMPOSITE of AgX ZEOLITE WITH CARBONIZED POLYANILINE FOR ELECTROANALYTICAL SENSING OF PHENOL COMPOUNDS**

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Ag⁺ cation-exchanged X zeolite was prepared by ion-exchange procedure and characterized by chemical analysis and scanning electron microscopy. The zeolite was subsequently used for the preparation of a composite with carbonized polyaniline. The electroanalytical response of the composite in the presence of phenol compounds (phenol, p-nitrophenol, and p-aminophenol) in acidic media was studied by voltammetric techniques. The results indicate that the composite electrode is suitable for phenol and p-nitrophenol sensing in aqueous media, while no response was obtained in p-aminophenol presence.

E-06-P**ELECTROCHEMICAL OXIDATION AND INTERACTION OF NEWLY SYNTHESIZED ACRIDINE DERIVATIVES WITH DNA**

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Oxidation of newly synthesized acridine derivatives was studied using cyclic voltammetry at glassy carbon electrode. Oxidation occurs as irreversible, diffusion-controlled process at pH 4.6 for compounds 1-3 and as adsorption controlled process for compound 4. The interaction between newly synthesized acridine compounds (compounds 1-4) and dsDNA was studied using a multilayer dsDNA biosensor applying square wave voltammetry. Peak current corresponding to deoxyadenosine decreased after 30 minutes of interaction suggesting interaction with dsDNA.

E-07-P**THE SYNTHESIS AND CHARACTERIZATION OF ZnMn₂O₄ IN AN AQUEOUS SOLUTION OF ZnCl₂**J. Senćanski¹, N. Nikolić², S. Blagojević¹ and I. Stojković Simatović³¹*University of Belgrade, Institute of General and Physical Chemistry,**Studentski trg 12-15, 11000 Belgrade, Republic of Serbia (sencanskijelena@yahoo.com)*²*University of Belgrade, Institute for Multidisciplinary Research, Kneza Višeslava 1, 11030 Belgrade, Republic of Serbia*³*University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-15, 11000 Belgrade, Republic of Serbia*

This work provides the synthesis and characterization of ZnMn₂O₄ that may be a potential replacement for the hazardous cathode materials used in commercial Li-ion batteries, as well as the examination of its electrochemical properties in an aqueous solution of ZnCl₂. Due to the fact that commercial Li-ion batteries contain toxic and flammable electrolyte, there is a need for their replacement with less harmful substance.

E-08-P**HYDROGEN EVOLUTION AT NICKEL/NICKEL OXIDE/CARBON COMPOSITES ELECTROCHEMICALLY PREPARED IN ALGINATE SOLUTION**J. Rupar¹, Aleksandra Janošević Ležaić¹ and N. Gavrilov²*University of Belgrade, Faculty of Pharmacy, ¹Department of Physical Chemistry and Instrumental Methods (jelena.rupar@pharmacy.bg.ac.rs)*²*University of Belgrade, Faculty of Physical Chemistry, Studentski Trg 12-15, 11000 Belgrade, Serbia (gavrilov@ffh.bg.ac.rs).*

In this work, carbon materials enriched in nickel (Ni) and nitrogen (N), obtained by carbonization of electrochemically synthesized alginate-based gels, were analyzed in 1 M potassium hydroxide (KOH) to assess their catalytic activity towards hydrogen evolution reaction (HER). SEM and elemental analysis confirmed the presence of Ni in all samples. Electrochemically active surface area (ECSA) was obtained from measured cyclic voltammograms (CVs), namely characteristic Ni²⁺/Ni³⁺ oxidation/reduction transition in synthesized composite materials. Sample Ni5AlgRiv, which in addition to Ni, contains a small percentage of N, dominantly formed by β-Ni(OH)₂, showed highest electro-catalytic activity for HER, with currents reaching few mA/cm².

*F - Biophysical Chemistry, EPR
Investigations of Bio-systems*

F-01-S**ROLE OF PRO-INFLAMMATORY S100 PROTEINS IN
AMYLOID-NEUROINFLAMMATORY CASCADE IN
NEURODEGENERATIVE DISEASES.**

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The amyloid cascade is central for the neurodegeneration disease pathology, including Alzheimer's and Parkinson's diseases, and remains the focus of much current research. Increasing evidence has accumulated demonstrating critical role of pro-inflammatory S100A9 in the amyloid-neuroinflammatory cascade in these diseases. We have demonstrated that S100A9 protein is intrinsically amyloidogenic and able to form amyloids both *in vitro* and *in vivo* in cell models and in neurodegenerative diseases. In Alzheimer's disease, deciphering the interaction between proinflammatory S100A9 protein and A β peptide and their co-aggregation mechanisms are particularly important since these lead to amyloid plaques formation and neural cytotoxicity. By using the combination of mass and charge distributions of amyloids together with reconstruction of the differences between them and detailed microscopy reveals that co-aggregation involves templating of S100A9 fibrils on the surface of Abeta42 amyloids. Kinetic analysis further corroborates that the surfaces available for the Abeta42 secondary nucleation are diminished due to the coating by S100A9 amyloids, while the binding of S100A9 to Abeta42 fibrils is validated by a microfluidic assay. We demonstrate that synergy between charge detection mass spectroscopy, microscopy, kinetic and microfluidic analyses opens new directions in interdisciplinary research.

Interactions of S100A9 with small molecules as potential regulators of its amyloid aggregation and functions, including interactions with NCAM1 peptide constructs, oleuropein aglycone, polyoxometalates and DOPA-derivatives, are discussed in the light of their potential therapeutic applications.

F-02-O**ANTIOXIDANT ENZYMES IN BLOOD OF WOMEN WITH UTERINE
HYPERPLASIA**

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The literature emphasizes the involvement of oxidative stress in the etiopathogenesis of many uterine diseases. Antioxidant system (AOS) represents the protective mechanism used by cells to neutralize overproduced reactive oxygen species (ROS) and prevent oxidative stress. We have previously shown that in gynecological patients with various diagnoses, the reproductive and other factors may be associated with antioxidant capacity and the ability to defend against oxidative damage. In this study, we examined the changes in expression of antioxidant enzymes (AOE): superoxide dismutases

(SOD), catalase (CAT), glutathione peroxidase (GPx), and glutathione reductase (GR) in the blood of women with endometrial hyperplasia. Our results indicate that hyperplasia induces perturbation in oxidative balance, particularly in glutathione redox cycle enzymes.

F-03-P**FTIR ANALYSIS OF XYLEM VESSEL CELL WALLS IN TWINING STEM OF *Dioscorea balcanica***

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Using stem cross sections of *Dioscorea balcanica*, as a model, we detected changes in anatomy and structural organization of xylem vessel cell walls (CWs) linked to stem twining in liana plants. UV microscopy, scanning electron microscopy and Fourier transform infrared (FTIR) microspectrometry were used. Different microfibrils orientation in vessel CWs of twisted compared to straight internodes, revealed by histological examination, coincide with the lower lignin content, the lower amount of xylan and cellulose, and the higher amount of xyloglucan, showed by FTIR. Xylem vessels resist high mechanical strain developed in twisted internodes by decreased CW rigidity (lower lignin content) and extensibility (higher xyloglucan content), and increased elasticity (lower xylan content).

F-04-P**INVESTIGATION OF THE SCAVENGING POTENCY OF SELECTED NEUROTRANSMITTERS AND THEIR METABOLITES TOWARDS IMIDAZOLYL RADICALS**

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The antiradical potency of several neurotransmitters and their metabolites – dopamine, 3,4-dihydroxyphenylacetic acid (DOPAC), catechol, 3-methoxytyramine (3-MT), and homovanillic acid (HVA), with water as a solvent, towards substituted imidazole radicals, was investigated according to three most common mechanisms. By calculating the enthalpy of reaction for each suggested mechanism, using thermodynamic parameters obtained through DFT simulations, the preferred reaction mechanism was determined for each molecule.

F-05-P**FLAXSEED OIL PREVENTS TRIMETHYLTIN-INDUCED UP-REGULATION OF ECTONUCLEOTIDASES ACTIVITIES IN THE RAT HIPPOCAMPUS**

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This study aimed to investigate the effects of trimethyltin (TMT)-induced hippocampal neurodegeneration and the beneficial effects of flaxseed oil (FSO) consumption on ectonucleotidase activities in the hippocampus of female rats. Animals were pretreated with FSO (1 ml/kg, orally) for two weeks then received a single dose of TMT (8 mg/kg, i.p.), and application of FSO continued for twenty-one days. Data have shown that FSO prevented TMT-induced up-regulation of ATP/ADP hydrolysis rates, while AMP hydrolysis remained unchanged in all examined groups. These findings support beneficial neuroprotective properties of FSO against TMT-induced neurotoxicity and hint at a promising preventive use of FSO in hippocampal degeneration and dysfunction.

F-06-P**ORAL D-GALACTOSE INTAKE PROVOKES REGION-SPECIFIC CHANGES OF GLUTAMATERGIC SIGNALING COMPONENTS IN THE BRAIN OF ADULT MALE WISTAR RAT**

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Extended lifespan highlights brain aging as an emerging worldwide problem. D-galactose (d-gal) is broadly used in animal aging studies as its chronic administration mimics aging-associated alterations, such as cognitive impairment in humans. This age-related cognitive impairment may be associated with alteration in synaptic structure and function, including changes in the glutamatergic system. Hence, we examined the effects of 6-weeks oral d-gal intake (200 mg/kg and 500 mg/kg) on protein expression of components involved in glutamatergic signaling in the prefrontal cortex (PFC) and hippocampus (HIP) of adult male Wistar rats. Decreased levels of vesicular glutamate transporter 1 (vGlut1) and NMDAR 2B subunit (NR2B) and a downward trend of postsynaptic density protein 95 (PSD-95) were observed solely in the PFC. Investigated components in the HIP were only slightly modified. These findings suggest the need for further research regarding region-specific glutamate involvement in age-related changes.

F-07-P**INVESTIGATION OF STRUCTURAL AND CONFORMATIONAL CHANGES IN Na/K-ATPase INDUCED BY DECAVANADATE**B. P. Bondžić¹, Z. Džambaski¹, T. Parac Vogt², A. M. Bondžić³¹ *Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia*² *Department of Chemistry, KU Leuven, Celestijnenlaan 200F, Leuven, Belgium*³ *Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11000 Belgrade, Serbia (aleksandrab@vin.bg.ac.rs)*

The decavanadate compounds (V10) have strong anticancer activity that is not yet fully understood. However, the cell proliferation seems to impact P-type ATPases. In this paper insights into structural and conformational changes of Na/K-ATPase induced by decavanadate were obtained using CD and 51V NMR spectroscopy. The CD measurements indicated the changes in α helix content and increase in disordered after addition of increasing concentration of decavanadate. 51V NMR spectra indicated the interaction of the enzyme with a specific vanadate species. The changes of the correspondent vanadate NMR signals were reflected in the broadening of the observed V10 NMR signals and changing of ratio of characteristic peaks. New peak was observed in 51V NMR spectra and was ascribed as vanadate–sucrose complex.

F-08-P**KINETICS OF ADSORPTION OF THE BOVINE SERUM ALBUMIN ON THE SILVER NANOPARTICLES**A. M. Bondžić¹, D. Jovanović², A. R. Leskovac¹, Z. Džambaski³, B. P. Bondžić³¹ *Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11000 Belgrade, Serbia*² *Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12–16, 11000 Belgrade, Serbia*³ *Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia (aleksandrab@vin.bg.ac.rs)*

In this study, the kinetics of bovine serum albumin (BSA) adsorption from aqueous solutions on the methionine stabilized silver nanoparticles (AgNPs) was investigated. The influence of the parameters such as contact time and BSA initial concentration on the adsorption capacity of AgNPs were tested. By increasing the contact time up to 30 min, the percentage of adsorbed BSA was increased. After this time, no changes were observed, indicating that the equilibrium state was reached. Investigation of the initial concentration-effect showed that the percentage of BSA adsorption increased with increasing BSA concentration until the available binding sites were saturated. After that, more BSA molecules were left unadsorbed. To elucidate the adsorption kinetic, pseudo-first-order, pseudo-

second-order, and intraparticle diffusion kinetic models were applied. The pseudo-second-order well described the adsorption process and intraparticle diffusion model rate laws, and the intraparticle diffusion is the sole rate-controlling step.

F-09-P

INFLUENCE OF ULTRAVIOLET B (UV-B) IRRADIATION ON ANTIOXIDANT CAPACITY AND FLUORESCENCE CHARACTERISTICS OF SOYBEAN (*GLYCINE MAX* L.) SEEDS

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UV-B light, plays a crucial role as a signal for inducing plant response and development of specific photomorphogenic responses. The UV radiation may have a damaging effect on cellular components and macromolecules in seeds, which may influence seed quality. We compared *Glycine max* L. seeds exposed to UV-B radiation for 1 h with non-irradiated seeds (control). The antioxidant activity was estimated using a DPPH assay. The seeds' fluorescence characteristics were studied by fluorescence excitation-emission matrices. According to the obtained results the UV-B irradiated seeds possess a significantly higher free radical scavenging activity compared to the control. The fluorescence analysis showed differences in the spectral emission profiles of irradiated seeds compared to the control seeds. The results imply that 1h seed exposure to UV-B increases free radical content which may alter the structures of cellular macromolecules resulting in degradation of some of the fluorophores.

F-10-P

CHEMICAL MODIFICATION OF HEMICELLULOSE ISOLATED FROM CORNCOBS TO OBTAIN HYDROGEL FOR ENZYME IMMOBILIZATION

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Hemicellulose rich in xylan was isolated from corncobs. Functional groups were introduced first by carboxymethylation and then by coupling with tyramine via carbodiimide-mediated reaction. Obtained hydrogel was tested for horseradish peroxidase (HRP) immobilization within microbeads, formed in an emulsion based enzymatic polymerization reaction. This model system showed that modified hemicellulose isolated from corncob is a suitable candidate for enzyme or small molecule immobilization for different purposes.

G - Organic Physical Chemistry

G-01-P**ANTIRADICAL POTENCY OF CYNODONTIN TOWARD HYDROXYL RADICAL**

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The antioxidant potency of cynodontin was studied in the presence of one of the most reactive free radical species, hydroxyl radical. This *in silico* study was done at the M06-2X/6-311++(d,p) level of theory. The geometry optimizations are performed in water and benzene, with an aim to simulate the polar and non-polar environment. The antiradical action of cynodontin *via* hydrogen atom transfer (HAT) and radical adduct formation (RAF) were determined.

G-02-P**ANTIRADICAL ACTIVITY OF FOLIC ACID TOWARDS •OH AND •OOH RADICALS**

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Folic acid have been investigated theoretically for its ability to scavenge hydroxy and hydroperoxy radicals. Reaction enthalpies for the reaction of these molecules with selected radical species, related to three mechanisms of free radical scavenging activity (HAT, SET-PT and SPLET), are calculated using B3LYP-D3BJ/6-311+G(d,p) level of theory. Calculated energy requirements indicated preferred radical scavenging mechanisms in polar (water) and non-polar (benzene) solvents. Both mechanisms, HAT and SPLET, are suitable for reaction FA with •OH in all solvents under investigations. On the other hand, in the reaction FA with •OOH, the SPLET is possible mechanism in both solvents.

G-03-P**POTENTIAL INHIBITORY EFFECT OF COUMARIN PALLADIUM (II) COMPLEXES ON SARS-CoV-2 MAIN PROTEASE**

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In this study, the inhibitory effect of the two previously synthesized palladium (II) complexes with chlorido-[(3-(1-(2-hydroxypropylamino)ethylidene)-chroman-2,4-dione)] and chlorido-[(3-(1-(2-mercaptoethylamino)-ethylidene)-chroman-2,4-dione)] on the SARS-CoV-2 main protease was evaluated. The investigation was carried out using molecular docking simulation. The results of this investigation indicate a potential inhibitory activity of coumarin derivatives on the SARS-CoV-2 main protease. Detailed description interactions between investigated compounds and protein can assist in the design of more specific and more potent antiviral drugs that can arrest the virus life cycle and progression of COVID 19 disease.

G-04-P

THE BARRIERS TO ROTATION AROUND THE C=C BOND BY THE MEANS TO QUANTIFY THE PUSH-PULL EFFECT OF THE BROADER SERIES OF SELECTED 2-ALKYLIDENE-4-OXOTHIAZOLIDINES UNDER DIFFERENT SOLVENT CONDITIONS

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In our previous work, based on the experimental and theoretical data of barriers to rotation around the C=C double bond of thiazolidine (*Z*)-**1a**, (*2E*, *5Z*)-**1e**, and (*E*)-**2b** that are determined under different solvent conditions, we showed that the *push-pull* effect of these compounds is not affected by the solvent (at least the two solvents studied). As the continuation of these studies, in this work we applied the same calculation procedure as we did for the (*Z*)-**1a**, (*2E*, *5Z*)-**1e**, and (*E*)-**2b** (solvents studied: chloroform and DMSO) to determine ΔG^\ddagger of (*Z*)-**1b**, (*Z*)-**1c**, (*Z*)-**1d**, (*Z*)-**2a** and (*Z*)-**2c** (solvents studied: chloroform and DMSO) as well as of **1-2** (solvent studied: water). All these results showed that barriers to rotation (ΔG^\ddagger) proved to be an excellent parameter by the means to quantify the *push-pull* effect of selected thiazolidines under reliable experimental conditions.

G-05-P**THE ENTHALPY–ENTROPY COMPENSATION MECHANISM OBSERVED
IN THE CONFIGURATIONAL ISOMERIZATION OF SELECTED 2-
ALKYLIDENE-4-OXOTHIAZOLIDINES UNDER THE SAME AND
DIFFERENT SOLVENT CONDITIONS**

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The results of our previous work showed that barriers to rotation (ΔG^\ddagger) around the C=C double bond of thiazolidine derivatives (*Z*)-**1**, (*2E*, *5Z*)-**2**, and (*E*)-**3** can be employed as the very efficient parameter to quantify their *push–pull* effect under different solvent conditions. We explained this by enthalpy–entropy compensation (EEC), occurring on the relationship: weak polar solvent (CDCl₃)/polar solvent (DMSO-*d*₆). In this paper, it has been at the first time demonstrated that the thermodynamics of C=C double bond rotation of the (*Z*)-**1**, (*2E*, *5Z*)-**2**, and (*E*)-**3** follows the EEC. Thus, a linear plot between their activation enthalpy (ΔH^\ddagger) and entropy (ΔS^\ddagger) has been observed, showing enthalpy–entropy compensation (EEC), which is occurred for both under the same solvent conditions and different ones. This result indicated that the ΔS^\ddagger and ΔH^\ddagger could be employed to quantify the *push–pull* effect of 4-oxothiazolidines under the same solvent conditions.

H - Material Science

H-01-O

PHYSICOCHEMICAL CHANGES OF BIMETALIC THIN FILM AFTER 300 fs/515 nm LASER IRRADIATIONS

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The method that enables highly controlled non-contact morphological and composition modifications of materials is laser processing. In the case of ultra-short laser pulses, as femtosecond (fs) ones, this method allows extremely accurate modifications, on micrometer and even on nanometer scale. Results concerning physicochemical changes after precise ablation of bimetallic thin film (BMTF), by single fs laser pulses, are presented. We investigated influence of the variations in pulse energy on composition and morphology changes. For used range of single pulse energies, we registered ablation of the upper layer of BMTF without ablation of the substrate.

H-02-O

GRAPH-THEORY APPLIED TO THE SOLID SKELETON EVOLUTION IN SINTERING

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Usually used methodology for modeling of microstructural evolution in sintering will be redefined by the introduction of the graph theory. Time- dependent evolution of graph data structure will be used for simulation of solid skeleton evolution induced by neck growth.

H-03-O**A NUMERICAL APPROACH TO ESTIMATE INTERGRANULAR CAPACITANCE IN CERAMIC SINTERING**B. M. Randjelovic and Z. S. Nikolic

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In this paper, a numerical method for predicting evolution of an intergranular capacitance during ceramic sintering will be defined. The contact between two grains undergoing sintering may be recognized as a structure that forms an intergranular capacitor whose capacitance changes as the neck grows by diffusion. It will be assumed that diffusion mechanisms responsible for material transport from the grain boundary to the neck are the volume and grain boundary diffusion only. The developed method will be applied for the computation of time-dependent intergranular capacitance during ceramic sintering of BaTiO₃ system.

H-04-O**OCHRATOXIN A AND ZEARALENONE ADSORPTION BY SURFACTANT MODIFIED ZEOLITE**

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Cetylpyridinium chloride (CP) was used to modify the surface of the natural zeolite and adsorption of two mycotoxins, ochratoxin A (OCHRA) and zearalenone (ZEN) was investigated. The organozeolites were prepared with three different levels of CP (20, 50 and 100% of zeolite's external cation exchange capacity) and mycotoxin adsorption experiments were done at pH 3 and 7. Results showed that with increasing amounts of CP at the zeolitic surface, adsorption of OCHRA and ZEN increased, as well as with increasing amounts of solid phase in suspension. Adsorption of OCHRA was dependent of the form of OCHRA in solution while ZEN adsorption was pH independent. Maximum adsorption was obtained with the highest level of CP present at the zeolitic surface for both mycotoxins.

H-05-O**CHEMICAL DOPING OF LANGMUIR-BLODGETT ASSEMBLED FEW-LAYER GRAPHENE FILMS WITH Li AND Au SALTS**

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To implement large-area solution-processed graphene films in low-cost transparent conductor applications, it is necessary to have control over the work function (WF) of the film. In this study we demonstrate a straightforward single-step chemical approach for modulating the WF of graphene films with Li and Au salts. Li-based salts decrease the work function, while Au-based salts increase the work function of the entire film. As a result, this method allowed to tune the WF of graphene electrodes in a range of 0.7 eV.

H-06-P**INFLUENCE OF COBALT LOADING ON THE PHYSICAL-CHEMICAL PROPERTIES OF PILLARED CLAY - SUPPORTED COBALT**

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The aluminum pillared clay (AP) was synthesized and impregnated with various cobalt loadings (x%CoAP, x=1, 3, 5, and 10 wt.%) by incipient wetness impregnation method. All samples were characterized by using X-ray powder diffraction (XRPD), inductively coupled plasma optical emission spectroscopy (ICP-OES) and low temperature N₂ physisorption techniques. The chemical analysis confirmed the successful incorporation of cobalt in all impregnated samples. Nevertheless, only cobalt oxide (Co₃O₄) was identified for samples having higher cobalt contents. Furthermore, different cobalt loading was mainly affected the microporous region in such way that micropore surface area decreased with the increase of cobalt.

H-07-P**MULTIFUNCTIONAL NANOCOMPOSITES BASED ON POLYMERS AND Ag NANOPARTICLES DESIGNED FOR DIFFERENT PURPOSE**

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In series of *in situ* aniline oxidative polymerization processes by silver ions (Ag⁺), and in the presence of polyvinylpyrrolidone (PVP) as an accelerator and stabilizer, six different SilverPolyaniline/Polyvinylpyrrolidone (AgPANI/PVP) nanocomposites were synthesized. With the variations in the synthetic conditions – pH adjustment, diversity in solvents, and molar ratios between components, differences in nanocomposites' structures, i.e., silver nanoparticles' (AgNPs) sizes and shapes, and PANI morphologies, were observed. Despite the same reactants are used in all polymerization processes, their direction/establishment are determined by environment (solvent, pH, reactants' concentrations) and components' oxidation potentials. These fast, simple and repeatable reactions yielded in dark powders, with differences in Ag content. As easily redispersible in water, these nanocomposites could find their value in the field of electrochemistry and/or as antimicrobial agents.

H-08-P**MODIFIED CHITOSAN FOR RAPID FABRICATION OF MICROLENSES**

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Chitosan was modified to prepare elastic, biocompatible, nontoxic, and ecofriendly material (MC) for rapid fabrication of microlenses. Concave, convex, aspheric microlenses (individual or arrays) are produced on the MC layer by direct laser writing at 488 nm. Microlenses can be used directly without chemical processing for different applications such as: medicine, sensors, cameras, security...

H-09-P**SYNTHESIS OF CORE-SHELL NaYF₄:Yb,Tm@TiO₂-Acac MICRO- AND NANO-SIZED PARTICLES FOR EFFICIENT PHOTOCATALYSIS**

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Micro- and nano-sized core-shell particles for efficient photocatalysis were successfully synthesized by a two step wet-chemical route. The core composed of up-converting (UC) NaYF₄:Yb,Tm phase was prepared through EDTA assisted hydrothermal process, while the shell of anatase TiO₂ – Acetylacetonate (TiO₂-Acac) charge-transfer complex was formed *via* a sol-gel method. During coating, the effect of polyvinylpyrrolidone (PVP) addition on the core and shell coupling was investigated. Two forms of core structures were obtained: hexagonal microprisms of β-NaYF₄:Yb,Tm and α-NaYF₄:Yb,Tm nanospheres, both coated with TiO₂-Acac nanocrystals.

H-10-P**THERMALLY INDUCED PHASE TRANSFORMATIONS AND THEIR INFLUENCE ON FUNCTIONAL PROPERTIES OF MULTICOMPONENT Fe-BASED AMORPHOUS ALLOYS**

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In this work, results of the study of five multicomponent iron-based amorphous alloys are summarized and compared regarding their thermal stability, mechanism of thermally induced microstructural transformations and their effect on the functional properties of the alloys. The obtained informations can be significant for development of the materials with targeted properties.

H-11-P**INFLUENCE OF POLYOXOPALLADATES(II) ON ECTO-NUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASES**

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Polyoxopalladates (POPs) are discrete, anionic palladium(II)-oxo nanoclusters combining properties of polyoxometalates and palladium(II), and thus are highly promising for the development of novel antitumor metallodrugs. The aim of this study was to investigate *in vitro* the influence of three POP salts with approved anti-neuroblastoma action, $\text{Na}_8[\text{Pd}_{13}\text{As}_8\text{O}_{34}(\text{OH})_6] \cdot 42\text{H}_2\text{O}$ (**Pd₁₃**), $\text{Na}_4[\text{SrPd}_{12}\text{O}_6(\text{OH})_3(\text{PhAsO}_3)_6(\text{OAc})_3] \cdot 2\text{NaOAc} \cdot 32\text{H}_2\text{O}$ (**SrPd₁₂**), and $\text{Na}_6[\text{Pd}_{13}\text{O}_8(\text{PhAsO}_3)_8] \cdot 23\text{H}_2\text{O}$ (**Pd₁₃L**), on E-NTPDase activity using rat synaptic plasma membranes (SPMs) isolated from *Wistar* brain as a model system. Dose-dependent inhibition of E-NTPDases was obtained within concentration range 2×10^{-6} - 1×10^{-3} mol/L for all investigated POPs. Inhibition parameters, IC_{50} value and Hill's coefficient, n_{H} , were determined by sigmoidal fitting the experimental results. The calculated IC_{50} values were $(1.08 \pm 0.25) \times 10^{-4}$, $(1.19 \pm 0.13) \times 10^{-4}$, and $(2.06 \pm 0.88) \times 10^{-4}$ mol/L for **Pd₁₃**, **SrPd₁₂**, and **Pd₁₃L**, respectively, indicating their similar inhibitory strengths. The n_{H} values were determined to be < 1 , indicating negatively cooperative binding for all POPs studied. The observed inhibitory effect of these anti-neuroblastoma POPs on E-NTPDase activity suggest that the inhibition of E-NTPDases, the enzymes representing the major part of purinergic signaling, could be considered as a putative mechanism of antitumor action and a new strategy in the development of novel antitumor therapeutics.

H-12-P**INHIBITION OF ECTO-NUCLEOSIDE TRIPHOSPHATE
DIPHOSPHOHYDROLASES BY POLYOXOPALLADATES WITH
PROMISING ANTILEUKEMIC PROPERTIES**M. B. Čolović¹, T. Ma², X. Ma², A. Isaković³, S. Misirlić-Denčić³, U. Kortz² and D. Z. Krstić⁴¹*Department of Physical Chemistry, "Vinča" Institute of Nuclear Sciences-National Institute of the Republic of Serbia, University of Belgrade, Serbia (colovicm@vin.bg.ac.rs)*²*Department of Life Sciences and Chemistry, Jacobs University, Bremen, Germany*³*Institute of Medical and Clinical Biochemistry, Faculty of Medicine, University of Belgrade, Serbia*⁴*Institute of Medical Chemistry, Faculty of Medicine, University of Belgrade, Serbia*

Polyoxopalladates(II) (POPs) are the largest subset of polyoxo-noble-metalates (PONMs), representing a class of discrete, anionic noble metal-oxo nanoclusters. In this study, the *in vitro* effects of two isostructural, fully inorganic POP salts containing tetravalent metal ions (Sn^{IV} and Pb^{IV}) incorporated inside the cubic Pd₁₂-oxo host-shell, Na₁₂[Sn^{IV}O₈Pd₁₂(PO₄)₈]·43H₂O (**SnPd₁₂**) and Na₁₂[Pb^{IV}O₈Pd₁₂(PO₄)₈]·38H₂O (**PbPd₁₂**), which were found to exhibit considerable antileukemic effects, on E-NTPDase activity were investigated using rat synaptic plasma membranes (SPMs) as a model system. Concentration-dependent inhibition of E-NTPDases was observed within the concentration range 5×10^{-6} - 2×10^{-4} mol/L for both POPs. Inhibition parameters, half-maximum inhibitory concentrations (IC₅₀ values) and Hill's coefficients, n_H, were determined by sigmoidal fitting the experimental results and Hill's analysis. The calculated IC₅₀ values were $(6.59 \pm 1.09) \times 10^{-5}$ and $(9.88 \pm 3.83) \times 10^{-5}$ mol/L for **SnPd₁₂** and **PbPd₁₂**, respectively. The calculated n_H values were < 1, indicating negatively cooperative enzyme-inhibitor binding for both POPs. Accordingly, the confirmed antileukemic activities of **SnPd₁₂** and **PbPd₁₂** could be associated with the observed inhibition of E-NTPDases as a potential target of the antileukemic action of these promising drug candidates.

H-13-P**CYTOGENOTOXICITY ASSESSMENT OF POLYOXOPALLADATES(II) AS
PROMISING ANTILEUKEMIC DRUG CANDIDATES**M. B. Čolović¹, G. Gajski², M. Gerić², T. Ma³, X. Ma³, U. Kortz³ and D. Z. Krstić⁴¹*Department of Physical Chemistry, "Vinča" Institute of Nuclear Sciences-National Institute of the Republic of Serbia, University of Belgrade, Serbia (colovicm@vin.bg.ac.rs)*²*Institute for Medical Research and Occupational Health, Zagreb, Croatia*³*Department of Life Sciences and Chemistry, Jacobs University, Bremen, Germany*⁴*Institute of Medical Chemistry, Faculty of Medicine, University of Belgrade, Serbia*

Polyoxopalladates(II) (POPs) are discrete, anionic palladium(II)-oxo nanoclusters that possess features of both conventional polyoxometalates (POMs) and palladium(II), which were shown to exhibit promising antitumor properties. In this study, *in vitro* cyto- and genotoxicity evaluation was

performed on normal non-target human blood cells using two isostructural POPs with tetravalent metal ions (Sn^{IV} , Pb^{IV}) encapsulated in the cuboid $\text{Pd}_{12}\text{-oxo}$ host, $\text{Na}_{12}[\text{SnO}_8\text{Pd}_{12}(\text{PO}_4)_8]\cdot 43\text{H}_2\text{O}$ (**SnPd₁₂**) and $\text{Na}_{12}[\text{PbO}_8\text{Pd}_{12}(\text{PO}_4)_8]\cdot 38\text{H}_2\text{O}$ (**PbPd₁₂**), with confirmed *in vitro* antileukemic actions against HL-60 cell line. For this purpose, whole blood samples were exposed to the POPs, at concentrations of $\approx \text{IC}_{50}$ (24 h) values, resulting in cytotoxicity in HL-60 cells for 24 h at 37 °C. The cytotoxicity studies were performed on human peripheral blood mononuclear cells which were stained with acridine orange and ethidium bromide, and then viewed under a fluorescence microscope. The genotoxicity was tested in whole blood by the alkaline comet assay (microgel electrophoresis). The results of the cytotoxicity evaluation and the comet assay demonstrated that none of the tested POPs, within the investigated concentration range 12.5 – 50 μM , resulted in a statistically significant modulation of blood cell viability as well as DNA damage, expressed as % of tail DNA (relative increase of tail DNA), compared to the untreated controls. Therefore, the promising antileukemic drug candidates, **SnPd₁₂** and **PbPd₁₂**, can be considered as selective and safe from a cytogenotoxicity point of view.

H-14-P

SILVER DODECATUNGSTOPHOSPHATE/BEA ZEOLITE ADSORBENTS FOR PESTICIDE REMOVAL

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Composite materials consisting of the silver salt of dodecatungstophosphoric acid and BEA zeolite are developed in order to obtain material with material of superior adsorption properties for pesticide removal from water. A two-step impregnation with variable constituent mass ratios was employed as a synthesis procedure. Composites are investigated by Fourier-transform Infrared (FTIR) spectroscopy, and results are compared with their adsorption capacities for glyphosate herbicide. A spectroscopic analysis reports the interaction of the BEA zeolite network with the silver salt of tungstophosphoric acid with evenly distributed adsorption sites in the investigated composites. The amount of glyphosate removed from water suspension was 243 mg/g of composite material.

H-15-P**IRON MODIFIED Y AND ZSM ZEOLITES AS PERSPECTIVE ECOFRIENDLY ADSORBENTS**

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This study investigated Y and ZSM-5 zeolites, important materials for a large number of different adsorption processes, modified with iron through an aqueous ion-exchange method, using dilute solutions of ferric citrate and ferrous oxalate. An Atomic Force Microscopy was employed for the analysis of zeolite microcrystalline surfaces. Acetamiprid, a neonicotinoid insecticide was chosen as a pollutant due to its extreme toxicity to bees and the negative impact on the environment. Characterization of material showed that crystal structure both zeolites is well defined and remained unchanged after the modification. Removal of acetamiprid from the water solution reached its maximum of 100 mg/g with Y citrate- and oxalate- modified samples, while citrate-modified ZSM-5 sample had the highest adsorbed amount of 38 mg/g.

H-16-P**SWELLING BEHAVIOR OF Ag-POLY(NiPAAm/IA) HYDROGEL NANOCOMPOSITES: INFLUENCE OF TEMPERATURE AND pH**

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In this work, swelling behavior of dual responsive Ag-poly(NiPAAm/IA) hydrogel nanocomposites, obtained by γ -irradiation induced synthesis, was investigated. Poly(NiPAAm/IA) hydrogels belong to the class of smart materials with thermo- and pH-sensitivity. Accordingly, swelling behavior was examined at two temperatures (25°C and 37°C) in three buffer solutions (pH 2.2; 4.5 and 6.8). Swelling and diffusion properties of investigated hydrogels were affected by polymer matrices composition, presence of AgNPs and environmental factors, such as temperature and pH of swelling media.

H-17-P**EFFECT OF SINTERING TEMPERATURE ON THE COMPRESSIVE STRENGTH AND MICROSTRUCTURE OF GLASS FOAM MADE FROM WASTE MATERIALS**

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Glass foams were produced from a green beer bottle and sugar beet factory lime (SBFL) as the foaming agent. The sintering temperature was in the 750-900 °C range. Porosity and compressive strength were determined. Results showed that glass foam sintered at 750 °C has the best compressive strength and even distribution of pores throughout the volume of the sample. With the increase of temperature from 800 to 900 °C compressive strength was improved while porosity has slightly dropped. Pores with diameters greater than 1000 µm were formed due to pore agglomeration. Obtained glass foams have properties comparable to commercial ones.

H-18-P**RADIOLYTIC SYNTHESIS AND CHARACTERIZATION OF ANTIBACTERIAL Ag-(PVA/PVP) HYDROGEL NANOCOMPOSITES**

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This paper describes the synthesis of nanocomposite systems of different compositions based on biocompatible polymers and antibacterial silver nanoparticles (AgNPs). The synthesis of hydrogel matrices of poly(vinyl alcohol) (PVA) and poly(*N*-vinyl-2-pyrrolidone) (PVP), as well as their combinations, was performed by gamma irradiation induced process. In the second step, *in situ* synthesis of AgNPs was performed by reducing silver ions, also using gamma irradiation, within previously synthesized matrices. Polymer matrices were characterized by swelling examination and scanning electron microscopy (SEM). The optical and microstructural properties of nanocomposites were analyzed by UV-Vis spectroscopy and X-ray diffraction (XRD), respectively. The antibacterial potential of the synthesized systems was confirmed by the diffusion test method on Gram-positive and Gram-negative bacteria.

H-19-P**THE INFLUENCE OF HYDROCHLORIC ACID ON THE FEATURES OF SBA-15 PARTICLES**

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The template method synthesis of both SBA-15 materials with elongated and spherical particles was performed using a surfactant Pluronic P₁₂₃. The HCl (p.a.) was used to synthesize material with elongated particles connected in chain structures grouped into shapes resembling sheaves of wheat. In the synthesis of spherical SBA-15 with diameters ranging from 0.5 to 2 μm, a spent HCl solution which was obtained after chemical treatment of clay was used where the dominant presence of the spheres was confirmed by the SEM method. In addition to the methods mentioned above, XRD, EDS and FTIR methods characterize SBA-15 materials.

H-20-P**MESOPOROUS SILICA DECREASE CELL VIABILITY *IN VITRO* IN DOSE DEPENDENT MANNER**

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Mesoporous silica renders chemical and mechanical stability under biological conditions, but due to its physicochemical properties, could be potentially harmful to exposed cells. The aim of the current study was to estimate SBA-15 (concentration of 50, 100 and 250 μg/mL) impact on human peripheral blood mononuclear cells to induce cyto- and genotoxicity *in vitro* after 72 h treatment, as well as lipid peroxidation in serum samples *ex vivo*. SBA-15 mesoporous silica treatment impact on cell viability was performed by XTT assay, lipid peroxidation was estimated by determining malondialdehyde and 4-hydroxyalkenals levels and genotoxicity by micronucleus assay. SBA-15 treatments displayed genotoxic potential at the lowest concentration, while highest tested concentration led to decrease of cell viability and increase of lipid peroxidation. Chemical modification of SBA-15 material that could influence its physicochemical properties could be useful way to lower its toxicity.

H-21-P**MICROWAVE ASSISTED SYNTHESIS OF POLYANILINE/PULLULAN (PANI/PULL) COMPOSITE**

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Microwave assisted synthesis of polyaniline modified by pullulan (PANI/Pull) composite was performed by aniline oxidation with potassium iodate. The PANI/Pull composite was characterized using ATR-FTIR technique. FTIR spectra confirm presence of both components in PANI/Pull composite. Antimicrobial evaluation of PANI/Pull material performed by using a qualitative disk diffusion method on *Candida albicans* (*C. albicans*) culture showed very high sensitivity to PANI/Pull composite. Observed FTIR and antifungal activity represent a promising results especially for potential biomedical applications of PANI/Pull composite.

H-22-P**SYNTHESIS AND CHARACTERIZATION OF NEW CERIUM DOPED PHOSPHATE TUNGSTEN BRONZE**

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Cerium doped phosphate tungsten bronze (Ce-PWB) was synthesized by phase transformations of CePW₁₂O₄₀×6H₂O (Ce-6-PWA) salt. The solid-solid transformations of Keggin's anion of this salt, including dehydration processes and bronze's formation are finished at about 600 °C. The

constructions of Ce-6-PWA and Ce-PWB were characterized by thermal analysis (TGA and DTA), X-ray powder diffraction (XRPD), and Fourier-transform infrared spectra (FTIR).

H-23-P

EVALUATION OF PERFORMANCE OF DISPERSION CORRECTED DENSITY FUNCTIONALS FOR TTF-TTF STACKING INTERACTIONS

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CCSD(T)/CBS energies for stacking interactions between two tetrathiafulvalene molecules were used as benchmark data to evaluate the performance of dispersion corrected density functionals in calculating the interaction energies. The results showed that the best functional for TTF-TTF stacking is B2PLYP-D3 with 6-311++G** basis set, which successfully reproduces gold standard CCSD(T)/CBS interaction energies. M06L-D3 functional with 6-311++G** basis set consistently underestimates interaction energies, giving potential energy curves of accurate shapes.

H-24-P

CHARACTERIZATION OF PRODUCTS OF PROLONGED HEMATOXYLIN AUTOXIDATION IN ALKALINE AQUEOUS SOLUTION

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The products of prolonged autoxidation of hematoxylin in alkaline aqueous solution were characterized by infrared (IR) spectroscopy, matrix-assisted laser desorption/ionization - time-of-flight mass spectrometry (MALDI-TOF MS), and electron spin resonance (ESR) spectroscopy. The IR data indicated that polymerization has occurred during this process. This was confirmed by the MALDI-TOF MS data, which also gave some insight into the degree of polymerization under our experimental conditions. The ESR data revealed that obtained products contain stable oxygen-centered radicals. This material has characteristics resembling natural and synthetic humic acid-like substances.

H-25-P**DIELECTRIC PROPERTIES OF PULSED LASER DEPOSITED NANOSCALE LaNi₅ THIN FILMS**R. Todoran, D. Todoran, Zs. Szakacs*Technical University of Cluj Napoca, North University Center of Baia Mare, Baia Mare, Maramures, Romania. (szakacsz@yahoo.com)*

Dielectric properties of pulsed laser deposited, nanoscale LaNi₅ alloy layers, on glass or SiO₂ substrate are described using the complex dielectric function. The UV-Vis-IR spectral behavior of this function is studied separately for its real ϵ_1 (the dielectric constant or dielectric permittivity), and imaginary part ϵ_2 (the dielectric loss function). The obtained absolute reflectance spectra were processed using the Kramers–Krönig formalism, so that the real and imaginary parts of the complex dielectric function could be computationally determined, also leading to the calculation of the electron loss functions $-\text{Im } \epsilon^{-1}$. This study reveals the layer thickness and deposition substrate dependent optical and electrical properties of the produced nanoscale LaNi₅ structures.

H-26-P**ALKYLAMMONIUM CLAY BASED NANOCOMPOSITES VS. ALKYLAMMONIUM-MODIFIED LIGNOCELLULOSIC MATERIALS IN ADSORPTION OF CONGO RED**N. Velić², M. Stjepanović², I. Ilić¹, M. Habuda-Stanić² and N. Jović-Jovičić¹¹*University of Belgrade – IChTM, National Institute, Center for Catalysis and Chemical Engineering, Njegoševa 12, 11000 Belgrade, Republic of Serbia (natasha@nanosys.ihtm.bg.ac.rs)*²*Josip Juraj Strossmayer University of Osijek, Faculty of Food Technology Osijek, Franje Kuhača 20, Osijek, Republic of Croatia*

In this study, lignocellulose waste materials and smectite clay were modified into adsorbents with surface free ammonium groups. Poplar waste biomass and brewer's spent grain were chemically modified. Smectite based adsorbents were obtained by intercalation of biopolymer chitosan and hexadecyl trimethylammonium (HDTMA⁺) cations in smectite structure. The samples were characterized by using X-ray diffraction, elemental analysis and FTIR spectroscopy. The adsorbents were tested for removal of azo dye Congo Red (CR). The concentration of CR was analyzed before and after adsorption test using Thermo Electron Nicolet Evolution 500 UV-VIS spectrophotometer in wavelength range from 250 – 800 nm. It was estimated that adsorption isotherms of CR for all investigated adsorbents showed best fit with Langmuir adsorption model.

H-27-P**KINETIC AND ISOTHERM STUDIES OF BIOSORPTION PROCESS OF COPPER IONS FROM WATER**

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The chemically modified lignocellulosic biomass with Al₂O₃ (LC-Al₂O₃) was tested as a new sorbent for the removal of copper (Cu(II)) ions from aqueous solution in batch conditions. As a lignocellulosic base material woodchips from an oak tree (*Quercus robur*) were used. To define the kinetic and equilibrium isotherm, experimental data were analyzed by pseudo-first-order and pseudo-second-order kinetic models and Langmuir and Freundlich isotherm models. Sorption kinetics followed pseudo-second-order model suggesting that surface reaction was the rate-limiting step. Equilibrium experimental results are the best fitted by the Langmuir isotherm model. The maximal sorption capacities of the biosorbent for removal of Cu(II) ions was 15.38 mg g⁻¹. According to the experimental data results, LC-Al₂O₃ seems to be an alternative and effective biosorbent for the removal of Cu(II) ions from aqueous solution.

H-28-P**THE EFFECTIVE REMOVAL OF REACTIVE DYE BY USING LAYERED DOUBLE HYDROXIDE**

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In this investigation, a layered double hydroxide (M-LDH) was synthesized by using the co-precipitation reaction. The morphology characteristics of the M-LDH were examined by SEM. It was found that the M-LDH was consisted of shards, nearly spherical particles with the size distribution of approximately 25 nm. The efficiency of the M-LDH for removal of reactive blue 19 (RB19) was evaluated by two parameters: contact time and initial dye concentration. The increase in contact time led to an increase in the sorption capacity, reaching equilibrium in approximately 120 min. The sorption capacity increased from 162.8 to 343.7 mg g⁻¹ with the increase in initial dye concentrations from 100 to 400 mg dm⁻³. Finally, the prepared M-LDH had the amenability to operate efficiently in the sorption of dyes from water.

H-29-P**DEGRADATION OF PESTICIDE 2,4-D WITH UV-ACTIVATED PEROXYDISULFATE AND HYDROGEN PEROXIDE**

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Two advanced oxidation processes based on combination of UV light irradiation with potassium peroxydisulfate and with hydrogen peroxide were employed for the degradation of pesticide 2,4-D in aqueous media. The influence of operating parameters, such as initial pH and concentration of the oxidant reagents, was investigated. Under the optimal operational conditions, complete degradation of pesticide 2,4-D was achieved after 15 and 30 min of treatments for UV/H₂O₂ and UV/S₂O₈²⁻ process, respectively.

H-30-P**CELL ADHESION CHARACTERISTICS OF POLYURETHANE-MESOPOROUS SILICA NANOPARTICLE COMPOSITE MATERIALS**

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Surface characteristics and biocompatibility of new nanocomposites based on polyurethane network and mesoporous silica nanoparticles (PUMSNs) were investigated. Surface topography and roughness coefficient were studied by AFM. Biocompatibility with endothelial cells and cytotoxicity of the PUNs were assessed using MTT (3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyl-tetrazolium bromide) and cell adhesion assays. The addition of MSNs into polyurethane network led to improvement of surface properties, as well as exhibited promising characteristics regarding adhesion of cells, toward potential application in coating for medical devices.

H-31-P**THERMAL CHARACTERIZATION OF POLYURETHANE/SILVER
FERRITE NANOCOMPOSITES**

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The novel polyurethane composite films were prepared using *in situ* polymerization method in the presence of silver ferrite nanoparticles (1 wt.%). Preparation, structure, and thermal characterization of polyurethane/silver ferrite nanocomposites (PUFNCs) were investigated. The study of the effect of soft segment content (from 30 to 60 wt.%) on the structure and thermal properties was performed using FTIR, DSC, TGA and TEM analyses. The higher thermal stability was detected for PUFNCs with higher soft segment content. The glass transition of the hard segment (T_{gHS}) of PUFNCs increased with decreasing soft segment content due to higher crosslinking density.

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Chemistry*

J-01-O**MODIFICATION OF TOKAT RESADIYE BENTONITE WITH CATIONIC SURFACTANT**

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The large bentonite reserves in Turkey are presently mined as very important raw materials for different industries. Application areas of bentonites vary, depending on kinds and amounts of its constituents such as smectites and non-clay minerals. In order to enhance the efficiency of Tokat Resadiye bentonite as a filler in polymer matrix, its modification with cationic surfactant, cetyltrimethylammonium bromide, was investigated in this study. The modified bentonite was examined by X-ray diffraction and Attenuated total reflectance fourier transform infrared spectroscopy.

J-02-O**FABRICATION of CS/PAA/Bnt as pH RESPONSIVE HYDROGEL FOR DRUG DELIVERY APPLICATIONS**

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The purpose of this work was to prepare Chitosan/Polyacrylic acid/Bentonite (CS/PAA/Bnt) as drug carrier for controllable drug delivery and highly-effective drug release. The materials used for preparation were bentonite (Bnt) clay, chitosan (CS) and acrylic acid (AA). The model drug for analyzing drug delivery and release kinetics was pantoprazole. The FTIR results confirmed that the drug active agent was successfully loaded into the prepared drug carriers. The swelling properties of the drug carriers were examined in buffer solutions at different pH values. The controlled pantoprazole release properties of the prepared samples showed that the release of the drug active reagent from drug carriers is pH-sensitive. The kinetics of the drug release was examined by fitting

the experimental data to the first order kinetic. CS/PAA/Bnt hydrogels were shown to be capable of carrying pantoprazole and can potentially be used in drug delivery systems.

J-03-P

SYNTHESIS AND CHARACTERIZATION OF EDTA FUNCTIONALIZED MACROPOROUS GLYCIDYL METHACRYLATE BASED COPOLYMER

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A novel functionalized macroporous poly(glycidyl methacrylate-co-ethylene glycol dimethacrylate), (pSGE-eda-EDTA) copolymer was obtained by two-step functionalization with ethylene diamine (EDA) and ethylenediaminetetraacetic acid (EDTA). The initial copolymers, as well as functionalized samples, were characterized by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), mercury porosimetry and elemental analysis. Additionally, the content of amino and carboxyl group, as well as the point of zero charge (pH_{PZC} value), were determined.

J-04-P

THERMAL PROPERTIES OF POLYURETHANE-CLAY NANOCOMPOSITES

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Two samples of poly(urethane-siloxane) nanocomposites (PUNs), based on 4,4'-diphenylmethane diisocyanate (MDI) and 1,4-butanediol (BD) as the comonomers of the hard segments (HS) and α,ω -dihydroxyethoxy propyl poly(dimethylsiloxane) (EO-PDMS) as the part of the soft segments (SS), were prepared by *in situ* polymerization. HS content of the prepared PUN samples were 10 and 20 wt%. Organomodified montmorillonite clay (Cloisite 30B[®]) was used as nanofiller (1 wt%) for

poly(urethane-siloxane)s. Prepared PUNs have good thermal stability, and they represent semicrystalline polymers.

J-05-P

**INVESTIGATION OF SORPTION BEHAVIOUR OF Cu(II) AND Pb(II)
ONTO A NOVEL EDTA MODIFIED COPOLYMER**

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A new metal-chelating glycidyl methacrylate based macroporous copolymer with ethylenediaminetetraacetic acid functions was tested as a potential Cu(II) and Pb(II) ions sorbent from aqueous solutions. The sorption was studied in non-competitive batch experiments, by varying initial pH and metal concentration, contact time and temperature. Pseudo-first and pseudo-second order model, as well as Bangham, intra-particle and liquid film diffusion models were used to determine the nature of sorption kinetics and the rate of limiting step. Equilibrium sorption data were analyzed with Langmuir, Freundlich, Temkin and Elovich isotherm models.

J-06-P

**POLYMER-SACCHARIDE CONJUGATES
I. THERMODYNAMICS OF TREHALOSE- LIVING CELL MEMBRANE
INTERACTIONS**

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This is the first in a series of papers, on unusual properties and high structural complexity of systems, based on conjugations of disaccharides with different polymeric entities, all been missed for a long time. Here we present interaction analyzes of trehalose, as living cell heat- and desiccation-protectant, in parallel with comparable features of trehalose 6-phosphate, and pullulan. Modeling and computer simulations, based on both main approaches- experimental, from yeast cell lines, and - theoretical, from thermodynamics, statistical mechanics and quantum-mechanics foundations of

modern physical chemistry, are presented. Here, at the start for the series, focus will be mainly on supramolecular structures of such systems.

J-07-P

**POLYMER-SACCHARIDE CONJUGATES
II. HEAT AND MASS TRANSFER THROUGH COATING-CELL
MEMBRANES OF PULLULAN FIBERS, SUPPORTED BY TREHALOSE
AND POSSIBLE APPLICATIONS IN VACCINE PRODUCTION**

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The results obtained in Part I indicate that for excellent cell protective effects obtained by trehalose, are required contributions of some additional substances involved in a kind of supramolecular structure with it, what has been proposed also by other authors, but what that can be, is unknown. To contribute solving the problem, we consider here possible role of pullulan, also used for protection by some fungi, but in completely different way.

J-08-P

**POLYMER-SACCHARIDE CONJUGATES
III. THE PROTECTIVE CONTROL OF CELL MEMBRANE ACTIVITIES
BY TREHALOSE WITH PULLULAN**

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Several possible protection mechanisms yeast cells use against desiccation, based on present theories and available experimental results are simulated, compared, evaluated, using molecular modeling, and analyzed in terms of present general theories on supramolecular polymer systems.

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

K-01-O

UPTAKE AND ACCUMULATION OF Pb AND Ni IN SPRUCE AND DOUGLAS-FIR TREE-RINGS AND BARK

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Modern development and increasing urbanisation, have production of a wide range of different pollutants, as a side effect. Trees in particular are emerging as an active factor receiving pollution. In a two-year study, we exposed spruce (*Picea abies* Karst.) and Douglas-fir (*Pseudotsuga menziesii* Mirb.) seedlings to elevated concentrations of Pb and Ni by adding these elements in the soil. Their concentrations as well as Mn and Zn concentrations in soil, tree-rings and bark were determined with Inductively Coupled Plasma- Optical Emission Spectrometry (ICP-OES). Analyses showed an increase of Pb and Ni in examined plant parts (tree-rings and bark) for both tree species, especially for Douglas-fir tree-ring.

K-02-O

ADSORPTION OF IBUPROFEN BY SURFACTANT MODIFIED KAOLIN

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In this paper, results of ibuprofen (IBU) adsorption by organokaolins obtained by modification of the natural kaolin (KR) with surfactant - hexadecyltrimethyl ammonium bromide (H) are presented. Two different amounts of surfactant were used for modification of KR (50 and 90% of kaolin's cation exchange capacity). Samples are denoted as HKR-50 and HKR-90. Adsorption of IBU on organokaolins was investigated with different initial drug concentrations (2 – 20 mg/L) in phosphate

buffer at pH 7. Compared with KR which has no affinity to adsorb IBU, modification of KR with H improved adsorption of this drug. Results showed that adsorption of IBU increased with increasing of the amount of surfactant in organokaolins as well as with increasing of the initial concentration of the drug in solution. Adsorption of IBU by both adsorbents followed nonlinear isotherms and from the Langmuir model, the maximum adsorption capacities were 2.05 mg/g for HKR-50 and 3.12 mg/g for HKR-90.

K-03-P

SOLID-PHASE EXTRACTION OF ESTROGEN HORMONES FROM WATER USING MULTI-WALLED CARBON NANOTUBES AS SORBENT

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Multi-walled carbon nanotubes were employed as a sorbent for solid-phase extraction of estrogen hormones (estrone, 17 β -estradiol, and 17 α -ethinylestradiol) from water solution. The solid-phase extraction (SPE) method was optimized by choosing an appropriate mass of the sorbent, volume, and initial pH of hormone water solution, as well as by choosing an appropriate organic solvent for extraction. Based on the obtained hormone recoveries, the following SPE conditions were chosen as optimal: 100 cm³ of hormone water solution at initial pH adjusted to 10; 20 mg of the sorbent; and methanol-dichloromethane mixture as elution solvent. Recoveries obtained under the optimal conditions ranged from 70.56 % for estrone, to 81.23 % for 17 α -ethinylestradiol, with a relative standard deviation from 9.92 to 18.74 %.

K-04-P

ENVIRONMENTAL RISK OF HEAVY METAL CONTAMINATION IN URBAN SEDIMENTS: A STUDY IN THE CITY OF BELGRADE, SERBIA

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Concentrations of 10 potentially toxic trace elements were measured in soil samples collected from 18 sites in urban areas of Belgrade, the capital and the largest city in Serbia. Samples were analysed in order to assess the extent of soil contamination and to distinguish natural and anthropogenic input. The results demonstrated a general Zn, Pb, and Cd enrichment in surface samples, hence, after comparison with guidelines, it has been determined that there is a potential risk for human health. In

the surface and buried samples, traces of copper were detected. The highest concentrations of Cr ($121 \pm 12.3\text{mg/kg}$) and Ni ($94.9 \pm 12.6\text{mg/kg}$) were found at a sediment depth of 2m and should be ascribed to geogenic sources. The results of HCA and PCA analysis supported a natural origin of Co, Cu, Mn, Cr, and Ni, while Cd, Zn, and Pb originated from anthropogenic inputs.

K-05-P

POLYCYCLIC AROMATIC HYDROCARBONS (PAHS) IN TWO HYDROGEOCHEMICAL DIFFERENT SEDIMENTARY ENVIRONMENTS OF THE TERTIARY KREPOLJIN BROWN COAL BASIN, SERBIA

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The sediments of the coal-bearing series of the Tertiary Krepoljin Brown Coal Basin have been investigated and presented in this manuscript. The samples of the intercalated mixed sediments (pieces of coal in clays, sandstones and shales) originate from two hydrogeochemically differing sedimentary environments: the illitemontmorillonitic (IM), and the calcitic (Ct) environment. The abundances of 16 polycyclic aromatic hydrocarbons (PAHs) on the priority list of the United States Environmental Protection Agency (U.S. EPA) have been determined in 10 analyzed sediment samples. The concentrations of Σ PAHs in sediments ranged from 449 to 10585 $\mu\text{g/L}$. A total of 8 of 16 PAHs, including B[a]A, Chry, B[b]F, B[k]F, B[a]P, IP, DB[a,h]A, and B[g,h,i]P, are regarded as potentially carcinogenic, indicating a higher possibility of occurrence of adverse ecological effect. High molecular-weight (HMW) PAHs are predominant in all sediments, but carcinogenic PAHs are predominant in sediments of Ct environment ($550\mu\text{gL}^{-1}$). Freshwater sediments show a lower sulfur content ($\Sigma 346 \pm 19.9 \mu\text{M/g}$ for IM samples, and $402 \pm 56.28 \mu\text{M/g}$ for Ct samples), with organic sulfur dominating. The molar ratio of H/C play a role in the changing process in the total PAHs, followed by the molar ratio of O/C and carbon content. Non-existence of the correlation between N/C ratio and other parameters indicates unspecific changes which accompany original terrestrial organic matter.

K-06-P

REMOVAL EFFICIENCY OF ARTIFICIAL SWEETENERS IN WASTEWATER TREATMENT PLANTS IN SERBIA

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Artificial sweeteners have been recognized as high-priority emerging contaminants that cause great concern due to unknown environmental behavior and long-term ecotoxicological impact on water resources. Wastewater treatment plants are not designed to remove these pollutants and consequently they are continuously introduced into the aquatic environment. This paper describes investigation of four artificial sweeteners, highly abundant in urban wastewater, and their removal rate in wastewater treatment plants in Serbia, in order to assess the efficiency of the treatment to reduce their environmental inputs. For this purpose, influent and effluent wastewater samples from two treatment plants were extracted and analyzed using liquid chromatography–tandem mass spectrometry.

K-07-P

VISCOSE-BASED ACTIVATED CARBON MATERIAL FOR MALATHION REMEDIATION

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Extensive use of the malathion invokes the development of efficient procedures for its elimination from the environment. Viscose-based activated carbon material was used for malathion removal from water. It was shown that 1 g of investigated material is capable to adsorb 0.727 g of malathion. Also, the toxicity of all samples was decreased after the treatment with the adsorbent.

K-08-P**GRAPHENE OXIDE AS AN ADSORBENT FOR DIMETHOATE REMOVAL FROM WATER**V. Anićijević¹, N. Potkonjak² and T. Lazarević-Pašti²¹ *University of Belgrade, Faculty of Physical Chemistry, Studentski Trg 12, 11000 Belgrade, Serbia.*² *University of Belgrade, VINČA Institute of Nuclear Sciences - National Institute of the Republic of Serbia, Mike Petrovica Alasa 12-14, 11000 Belgrade, Serbia. (lazarevictlj@yahoo.com)*

Nowadays, the use of organophosphate pesticide dimethoate is widespread. Dimethoate is toxic for mammals, so efficient procedures for its elimination from the environment are necessary. We used graphene oxide for dimethoate removal from water. It was shown that 1 g of investigated material is capable of adsorbing 8.8×10^{-3} mol of dimethoate. A satisfactory agreement of experimental results with the Langmuir isotherm model suggests the monolayer adsorption on the homogenous surface.

K-09-P**DOES HUMIFICATION TAKE PLACE DURING BIODEGRADATION OF PETROLEUM HYDROCARBON?**J. Avdalović¹, N. Lugonja¹, K. Joksimović¹, M. Lukić², J. Milić¹,
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The aim of this paper was to study using an active consortium of zymogenic microorganisms for *ex situ* biodegradation of a petroleum hydrocarbon, along with simultaneous monitoring of the humification process.

In this study, the biopile (B) and control biopile (CB) for *ex situ* bioremediation consisted of soil polluted with petroleum and its derivatives. The initial level of total petroleum hydrocarbon (TPH) in the B and CB was 26 g kg^{-1} . At the end of the study, TPH were reduced to 4 g kg^{-1} in B, but only to 24 g kg^{-1} in the CB. The starting material contained 2.79% of humic acids (HAs) while at the end of study, HAs in the B had increased to 3.88%, in contrast, in CB, only a very small increase of HAs, to 2.90% was noted. Also, the quality of humification was monitored by determining parameters such as HAs/FAAs (the humic acid/fulvic acid ratio) and HI ($C_{\text{HAs}}/\text{TOC}$).

The current results show undoubtedly that humification occurred during biodegradation of petroleum hydrocarbon.

K-10-P

DYNAMICS OF DIESEL BIODEGRADATION BY *PLANOMICROBIUM* SP ISOLATED FROM PETROLEUM CONTAMINATED SOIL

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A direct consequence of the use of fossil fuels is the environmental contamination during production, processing and distribution. Microbial biodegradation is efficient technique for cleaning contaminated areas which follows the principles of sustainability. This paper presents the dynamics of biodegradation of hydrocarbon fractions of diesel D2, using *Planomicrobium* sp. RNP01 isolated from the area contaminated with petroleum pollutants. The obtained results showed that after 30 days of biodegradation of diesel D2 significant degradation is achieved, with almost complete degradation of *n*-alkanes and decrease in the amount of sesquiterpane.

K-11-P

THE REDUCED COMPTON WAVELENGTH AND THE ENERGY-POSITION/MOMENTUM-TIME-UNCERTAINTIES

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The Compton scattering is an elastic collision of the x-ray or gamma photons with free electrons (or loosely bound valence shell electrons). This scattering is demonstrated in Fig. 1. In this communication, we are combining Heisenberg's uncertainty principle and the Compton scattering. Note, that some of the expressions (including their derivations) of this communication can be found in modern physics textbooks.

K-12-P**RADIOACTIVITY IN SOIL AND MOSSES FROM NP ĐERDAP IN 2019**

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In June 2019, 18 soil samples and 20 moss samples were collected from 3 regions on the territory of National Park Đerdap. The radionuclide content (Bq/kg) in soil (moss) was: ¹³⁷Cs 3.5-496 (5.5-908), ⁴⁰K 36.4-918 (136-493), ²²⁶Ra 7.8-45.0 (4.2-34.1), and ²³²Th 8.2-59.5 (1.7-22.2). The external gamma dose rate (nGy/h) in 2019 on the territory of NP Đerdap is in the range from 22.4 to 93.6, average value 50.0. Values of the external gamma dose were in the range of the expected values and close to the average values in the world. The mean value of annual effective dose (10^{-5} Sv) in the NP Đerdap is 6.12×10^{-5} and is lower than the mean value on the world level of 7.00×10^{-5} Sv.

K-13-P**MULTI-WAVELENGTH LIGHT ABSORPTION ANALYSIS OF BLACK CARBON IN FINE FRACTION OF SUBURBAN AEROSOL**

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A multi-wavelength light absorption of black carbon (BC) in fine aerosol particulate matter was analyzed to estimate BC contribution coming from different emission sources to receptor site in Banja Luka suburb. Analysis was performed at 140 daily PM_{2.5} samples collected on PTFE filters. Blank and exposed filters were irradiated by monochromatic light in range 405-1050 nm and related intensity attenuation due to absorption by BC present in aerosol deposits have been recorded. Obtained results and relationships between light- and mass- absorption coefficients and their dependence on the PM_{2.5} deposit characteristics allowed differentiation between BC dominantly coming from fossil fuel combustion and BC formed in biomass burning emissions that is valuable information for PMF receptor modeling.

K-14-P**IMPACT OF PHARMACEUTICAL LEVELS IN UNTREATED WASTEWATER ON BELGRADE RIVER WATER QUALITY**

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In the city of Belgrade, raw sewage is discharged directly into the Sava and the Danube rivers affecting the quality of river water. To determine the level of this impact, eight frequently used and detected pharmaceuticals were selected for the study. A previously developed method for analysis of pharmaceuticals in different water matrices was used. Sample extracts were analyzed by liquid chromatography-tandem mass spectrometry, using the electrospray ionization technique. The most commonly detected analytes in both municipal wastewater and surface water were carbamazepine, known for its high environmental stability, and diclofenac, known as having high acute ecotoxicity. The dilution effect, noted for most of the detected drugs, was not as pronounced with diclofenac, indicating a higher risk for aquatic organisms.

K-15-P**DOES EXPOSURE TO A SINGLE DOSE OF MICROPLASTIC REPRESENTS A HEALTH RISK?**

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Worldwide pollution with plastic debris represents tremendous environmental issue. Small particles originated from plastic bottles exert various effects in organisms when exposed chronically, while the effects of a single exposure are completely unknown. Thus, to test their potential health impact, male Wistar rats were exposed by oral gavage to a single dose of microplastic particles (MP) derived from polyethylene terephthalate (PET) bottles (1.4, 35 or 125 mg/kg with median diameter of 85 µm). Food and water intakes were monitored, and neurological and clinical tests were conducted. Obtained results point to lower food and water intakes in groups that received two higher MP doses indicating to interference with normal digestion. None of three used MP doses provoked neurological and clinical impairments either due to short-term exposure and/or lack of MP cumulative effect. Overall, presented results indicate that exposure to a single dose of MP can initiate health issues.

K-16-P**POTENTIAL USE OF SLAG GENERATED FROM LIGNITE COMBUSTION IN HITTING PLANTS**

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This paper presents the examination of potential application of slag, obtained from lignite combustion process in heating plant in Valjevo, Serbia, as a replacement for cement in mortars and concrete production. Waste slag was characterized with X-Ray Diffraction Analysis, Field Emission Scanning Electron Microscopy and Gamma spectrometric analysis, while its application possibility was investigated with testing Pozzolan activity Strength activity index, Activity index and Water requirement. The aim of this study is to determine under what conditions the slag could successfully replace cement in construction industry in certain percentages. Based on presented results it was concluded that, after mixing with silicate fume, waste slag can be used for the purpose mentioned. Optimal proportion of cement replacement is 20% -: 18% of slag and 2% of silica fume.

K-17-P**BLACK INORGANIC PIGMENTS OBTAINED FROM WASTE MATERIALS**

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Hazardous industrial wastes are the most common source of environmental pollution. Waters originating from unregulated landfills and places of inadequate disposal of this type of wastes can pollute the water sources and affect the human health. In this study, electroplating waste sludge (ES) and various Fe-rich wastes were used as starting materials for the synthesis of inorganic pigments. Obtained black $\text{Cr}_{1.3}\text{Fe}_{0.7}\text{O}_3$ pigments possess adequate properties required for use as inorganic pigments.

K-18-P**DEVELOPMENT AND VALIDATION OF A SPE-HPLC-DAD METHOD FOR THE DETERMINATION OF SELECTED PESTICIDES IN WATER SAMPLES**

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An analytical method based on solid-phase extraction (SPE) using coconut shell activated carbon (CSAC) as a low-cost adsorbent and high performance liquid chromatography with diode array detector (HPLC-DAD) was developed and validated for the determination of four varying polarity pesticides in water samples. SPE procedure was optimized and under the optimized conditions the proposed method was validated. The method exhibited good linearity, satisfactory precision (1.4 – 5.1%), high enrichment factor, good recovery and low limits of detection (0.025 – 0.039 $\mu\text{g}/\text{dm}^3$). Optimized method was used to determine selected pesticides in tap water samples. The recoveries ranged from 58.2% to 105.3%, with low relative standard deviations. The obtained results indicated that the proposed SPE-HPLC-DAD method could be efficiently used for the determination of the selected pesticides in environmental water samples at trace levels.

K-19-P**DEVELOPMENT OF CHITOSAN-BASED HYDROGEL BEADS FOR HEAVY METALS REMOVAL FROM AQUEOUS SOLUTIONS**

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Chitosan and its modified forms have received great attention as potential adsorbents due to its outstanding adsorption characteristics toward removal of various toxic heavy metal ions from aqueous solutions. In this work, porous chitosan hydrogel beads (CHB) and CHB cross-linked with glutaraldehyde (GLA) and citric acid (CA) were synthesized and used for investigation of its adsorption performances toward the removal of Pb(II), Cu(II), Zn(II), Cd(II) and Cr(VI) ions from water in batch and dynamic systems. Maximum removal was achieved in the pH ranges of 4.0 - 6.5 and 2.0 - 3.5 for divalent cations and Cr(VI) oxyanion, respectively. The equilibrium adsorption data were best fitted by the Langmuir isotherm model. Based on the optimal conditions, the fixed-bed breakthrough curves for the removal of the studied metal ions from the aqueous solutions using fixed-bed columns were experimentally evaluated, as well as theoretically predicted using COMSOL Multiphysics software.

K-20-P**PARTITIONING OF DIFFERENT POLARITY PESTICIDES,
DELTAMETHRIN AND DICAMBA, IN AQUEOUS BIPHASE SYSTEMS
WITH IONIC LIQUIDS**A. Jocić, S. Marić, J. Milićević and A. Dimitrijević*Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia
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An aqueous biphasic system (ABS) composed of the imidazolium and choline based ionic liquids mixed with potassium phosphate salt (K_3PO_4) was suggested as the ABS system suitable for extraction of two different polarity pesticides deltamethrin (DLT) and dicamba (DCM). The influence of two ionic liquid (IL) cations on the partitioning behavior of examined pesticides from aqueous solution was evaluated. The results showed that both pesticides, DLT and DCM preferably migrate to the more hydrophobic, IL-rich phase. The higher DLT partition coefficient was obtained for more hydrophobic imidazolium-IL enriched ABS phase ($\log K_{DLT}=2.59$) compared to ABS with choline IL ($\log K_{DLT}=2.25$). On the other hand, less hydrophobic DCM distributes more in the IL-rich phase of choline-based ABS ($\log K_{DCM}=0.85$) in relation to imidazolium-based ABS ($\log K_{DCM}=0.33$).

K-21-P**SYNTHESIS OF ACTIVATED CARBONS FROM WATER HYACINT
BIOMASS AND ITS APPLICATIONS AS ADSORBENTS FOR HERBICIDE
GLYPOSATE**A. Hakky Mohammad and M. Kijevcanin*University of Belgrade, Faculty of Technology and Metallurgy,
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In this work the activated carbons were synthesized from hyacinth biomass by chemical activation with $ZnCl_2$, followed by carbonization in temperature range from $400^\circ C$ to $700^\circ C$. The content of C, H and N was estimated by elemental analysis while the textural properties of samples were obtained from adsorption-desorption isotherms of N_2 at $-196^\circ C$. The obtained activated carbons were applied as adsorbents of herbicide glyphosate.

K-22-P**ISOLATION OF ACETAMINOPHEN FROM IONIC LIQUID RICH-PHASE OF THE AQUEOUS BIPHASIC SYSTEM**

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In this work, extraction of acetaminophen using an aqueous biphasic system and its isolation from the ionic liquid-rich phase through precipitation with the anti-solvents were studied. The obtained result show that system composed of 1-butyl-3-methylimidazolium chloride and copolymer is able to extract acetaminophen to ionic liquid phase. Also, the results indicate that the isolation of acetaminophen from ionic liquid phase is possible by the addition of potassium chloride in appropriate volume ratio. The results obtained can be used in the development of process for the recovery of valuable drugs from pharmaceutical wastes.

K-23-P**APPLICATION OF CHLORINE DIOXIDE FOR PHARMACEUTICAL DEGRADATION**

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This study investigated degradation of ibuprofen in deionized and river waters using chlorine dioxide treatment. The degradation degree of ibuprofen was monitored by high-performance liquid chromatography (HPLC) analysis. The toxicity effect of degradation products was determined by *Daphnia magna* bioassay. The results showed that alkaline condition favors the degradation of ibuprofen and high concentration of chlorine dioxide is required for very efficient degradation of ibuprofen. Degree of degradation in the real water sample is relatively low and ranged from 42% to 47% compared to the degree of degradation in deionized water (99%). The results of toxicity tests showed that degradation products of ibuprofen belong to class III as acutely toxic.

K-24-P**THE LIFETIMES OF ^{238}U NUCLEI, THE ESCAPING ATTEMPTS OF THEIR ALPHA PARTICLES AND THE GEIGER-NUTTAL LAW**

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We consider here the large populations of ^{238}U nuclei and their emitted alpha particles. The main points are: (a) a time interval for which alpha particle of ^{238}U nucleus makes one attempt to escape is approximately 10^{-21} second; (b) the number of the mean escape attempts is $\sim 2 \times 10^{38}$; (c) contribution of the tunneling time of ^{238}U nucleus to the mean time and to the lifetime of each individual nuclei is negligible; (d) the sum of the lifetimes of ^{238}U nuclei and the sum of the number of escape attempts of their alpha particles are constant. Consequently, the ratio of these two sums is also constant, and is about 10^{-21} seconds; and, (e) a new mathematical form of the Geiger-Nuttall law is derived using a very simple theoretical approach.

K-25-P**QUANTITATIVE DETERMINATION OF DEHP BY FOURIER TRANSFORM INFRARED SPECTROSCOPY**T. Anđelković¹, D. Bogdanović¹, I. Kostić¹, G. Nikolić², B. Kostić², and R. Pavlović³¹*University of Niš, Faculty of Science and Mathematics, Department of Chemistry, Višegradska 33, 18000 Niš, Serbia*²*University of Niš, Faculty of Technology, Department of Chemistry and Chemical Technology, Bulevar oslobođenja 124, 16000 Leskovac, Serbia*³*University of Milan, Department of Veterinary Science and Public Health, Via Celoria 10, 20133 Milan, Italy**(Corresponding author: e-mail: dannica.milojkovic@gmail.com)*

Phthalates are chemical substances that are widely used as plasticizers that are added to PVC to improve their properties. Because of phthalate tendency to migrate to environment and their harmful effect on human health, the aim of this paper is quantification of di(2-ethylhexyl)phthalate (DEHP) in PVC pharmaceutical contact materials (PCM articles) using Fourier transform infrared spectroscopy (FTIR). Quantification was performed based on obtained linear calibration curve for DEHP within the mass concentration range from 0 to 50% in relation to mass of PVC article for two monitored ranges on the FTIR spectrum ($720\text{-}760\text{ cm}^{-1}$ and $1560\text{-}1610\text{ cm}^{-1}$). The results showed that the investigated transfusion set and tubing for transfusion contains the most DEHP (27.50%), followed by quadrupole bag with 24.1%, transfer bag with 22.9% and sag-M bag for transfusion with 4.98%.

K-26-P

PHTHALATES DETERMINATION IN CHILDREN TOYS BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY

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The aim of this work was qualitative and quantitative determination of dimethyl phthalate (DMP), di-*n*-butyl phthalate (DnBP), benzyl butyl phthalate (BBP), di(2-ethylhexyl)phthalate (DEHP), di-*n*-octyl phthalate (DnOP) in plastic children toys using the GC-MS technique. Phthalates were isolated from the PVC toys by tetrahydrofuran and then polymer was precipitated by the addition of an excess of *n*-hexane. Based on presence or absence of peaks at the specific retention time in the obtained GC-MS chromatogram of PVC toys, the existence of phthalates in the PVC toys was checked. Based on the obtained calibration curve with correlation coefficient 0.999 for DEHP, the only phthalate qualitatively detected in toys, the mass percentage of DEHP in each toy was determined. The amount of DEHP in the 13 analyzed PVC toys was in the range from 9.47 to 53.24 % by weight of PVC article. The five analyzed PVC articles did not contain noted five tested phthalates, while one plastic toy was not made of PVC. The obtained results indicated that some children toys have high amount of DEHP, which certainly exceeds the allowable DEHP concentration.

K-27-P

INFLUENCE OF UV RADIATION TO DEHP CONCENTRATION IN PVC CHILDREN TOYS

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In order to determine the influence of UV-A and UV-C radiation on the structure of polymers in PVC toys, and therefore on the bond strength between DEHP and polymer, the concentration of DEHP in PVC toys was determined after irradiation of PVC toys using UV-A and UV-C light for a certain

period. After performed calibration, DEHP quantification in two irradiated PVC toys was done using GC-MS technique. The obtained results indicated that UV-A and UV-C light influenced on DEHP migration from PVC toys into environment, which further affected the decrease in DEHP concentration in PVC toys. With increasing duration of radiation of these toys, the mass concentration of DEHP in the toys decreased, and for toy 1 was decreased from 27.04 to 19.58 mass%, while for toy 2 this decrease was from 36.82 to 30.81 mass%.

K-28-P

CADMIUM TRANSLOCATION EFFICIENCY IN WATER LETTUCE

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Heavy metals commonly found in waters are As, Pb, Hg, Cd, Ni and Cr. The major cost of heavy metal pollution is their bioaccumulation. Phytoremediation of waters and soils refers to the use of pollutant-accumulating plants to extract and accumulate contaminants from contaminated medium. The main objective of this study was to estimate the translocation efficiency and response of *P. stratiotes* on increased cadmium levels in water. Estimation of translocation efficiency was performed for a nutrient-free water polluted with 1, 5, 10, 15 and 20 ppm of cadmium, over 15 days of growth. High translocation efficiency was observed for plants grown up to five days in water with the two lowest levels of tested cadmium contamination.

K-29-P**WASTE COTTON/POLYESTER YARN AS AN ADSORBENT FOR THE REMOVAL OF HEAVY METALS FROM WASTEWATER**

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Waste cotton/polyester yarn was used for the removal of Pb(II), Cd(II), Cr(III) and As(V) ions from aqueous solution. In attempt to increase the adsorption efficiency, cotton/polyester yarn was modified by sodium hydroxide solution. Characterization of examined yarns was performed by scanning electron microscopy, Fourier transform infrared spectroscopy and streaming potential method for determination of the isoelectric point. It was shown that applied treatments slightly affected the surface acidity due to increased availability of ester groups and changes in cellulose-derived groups. These changes in surface chemistry of modified cotton/polyester yarns did not improve their adsorption capacity for Cd(II), Cr(III) and As(V) ions. However, both unmodified and modified waste cotton/polyester yarns could be used for efficient removal of lead ions from wastewater.

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

L-01-P**NITROGEN DOPED CARBON CRYOGEL AS A SORBENT FOR HEAVY METAL IONS (ZN, CD, HG)**

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Heteroatom incorporated into carbon material structure may result an increase of specific surface area, amount of surface functional groups, formation of new functional groups and an increase of charge which are important for improvement of adsorption process. The aim of this work was to investigate possible application of nitrogen doped carbon cryogels (CCN) for heavy metals removal from waste water. Adsorption kinetics and influence of pH value on adsorption were investigated. In order to describe the adsorption mechanism on carbon cryogel, the adsorption isotherms were determined. The obtained results showed that the incorporation of nitrogen into the carbon cryogel structure leads to an increase in the specific surface area and oxygen content. Adsorption study showed that the samples with the highest concentration of incorporated nitrogen showed better adsorption characteristic and faster adsorption equilibria compared to undoped carbon cryogel. Also, pH decrease of water solutions leads to stronger π - π interaction between functional group on carbon surface and metal ions from solution that leads to a better metal removal from water.

L-02-P**INFLUENCE OF SEC-ALKAN SULFONATE ON DISHWASHING ANIONIC SURFACTANTS MIXTURE**

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Surface active properties and foamability of anionic surfactants mixtures (sodium lauryl ether sulfate (SLES), sec-alkan sulfonate (sodium C14–17 alkyl sec sulfonate (SAS)), cocamidopropyl betaine (CB) and cocodiethanolamide (DEA) were studied. Investigated features of particular anionic surfactants mixture were critical micelle concentration (CMC), surface tension (γ) and foam volume. The aqueous mixture composition, containing SLES, CB and DEA in ratio 10:1:0.5 (expressed in mass percent) were base anionic surfactants mixture. With the addition of SAS to the SLES/CB/DEA surfactants mixture, both CMC and γ were decreased, as well as foaming properties of SLES/CB/DEA were improved. All those indicate that SAS surfactant can be used to produce better cleaning products.

M - Complex Compounds

M-01-P**CRYSTAL STRUCTURE OF THE MACROCYCLIC COMPLEX
[Co₂(μ-pht)tpmc](ClO₄)₂·H₂O**

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The crystal structure of the Co(II) complex [Co₂(pht)tpmc](ClO₄)₂·H₂O (pht= phthalate dianion; tpmc= *N,N',N'',N'''*-tetrakis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane) was determined by X-ray diffraction method. The complex crystallizes in monoclinic crystal system, *C2/c* space group. The geometries around both Co(II) atoms are highly distorted octahedral. The Co(II) ions exhibit CoN₄O₂ coordination environments with the four nitrogen donor atoms of the tpmc ligand and two oxygen atoms belonging to the one carboxylate group of pht²⁻ ligand. The carboxylate groups of pht²⁻ are coordinated in an *endo*-bidentate mode. The tpmc ligand adopted a *boat* conformation in which the two coordinated Co(II) atoms are located on the same side of the ring, with Co···Co distance amounting 5.4799(5) Å.

M-02-P**STABILITY CONSTANTS OF FOUR BINUCLEAR Co(II) COMPLEXES
WITH A MACROCYCLE AND DIFFERENT CARBOXYLATO
CO-LIGANDS**

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The complexation reaction between Co²⁺ with the tpmc = *N,N',N'',N'''*-tetrakis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane and carboxylate/dicarboxylate co-ligands, was studied using spectrophotometric method. The stoichiometric composition and stability constants of four mixed-ligand Co(II) complexes of formulas [Co₂(benz)₂tpmc](ClO₄)₂ (**1**), benz⁻ = benzoate anion; [Co₂(L)tpmc](ClO₄)₂, L = pht²⁻ (phthalate dianion) (**2**), L = ipht²⁻ (isophthalate dianion) (**3**) and L = tph²⁻ (terephthalate dianion) (**4**) are reported. The stoichiometric ratio of the compounds was determined spectrophotometrically at 20 °C and constant ionic strength of 0.1 mol dm⁻³ (KNO₃) in ethanol–water mixtures as the solvent using Job's methods of continuous variation. The values of stability constants *K* and Gibbs free energy Δ*G* were calculated.

M-03-P

**EFFECT OF TRANS SUBSTITUENT ONTO HYDROGEN BOND
INTERACTION IN SQUARE-PLANAR PLATINUM (II) COMPLEXES**

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The influence of *trans* substituent onto hydrogen bond interaction energies was studied. The interaction energies for neutral, singly and doubly charged platinum(II) complexes with water molecule were calculated at M06L-GD3/def2tzvpp level. The results on interaction energies have shown that ligands in *trans* position to interacting water molecule does not show the same trend in different molecules.

N - General Physical Chemistry

N-01-S**APTAMER-SMALL-MOLECULE TARGET STRUCTURE-ACTIVITY
RELATIONSHIPS: FROM GROUP FREE BINDING ENERGY
CONTRIBUTIONS TO ELECTRON TRANSFER RATES**

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Aptamers (oligonucleotide-based receptors) are isolated from random libraries through cycles of enrichment based on binding to a target coupled with amplifications. There are two fundamental advantages of aptamers over antibodies: (1) We can select aptamers for small molecules ignored by the immune system even when haptened, *e.g.*, in the past we targeted neurotransmitters and amino acids and (2) Aptamers are readily engineered to undergo gross conformational changes upon ligand binding, which makes them perfect receptors for biosensor applications. However, despite these important advantages, clinical applications have been largely precluded by the paucity of aptameric receptors achieving clinically relevant affinities and specificity.

I will present our recent systematic studies using group free energy of binding contributions that led us to a comprehensive approach based on functional group analysis to overcome traditional barriers to isolation of high-quality aptamers. I will specifically discuss new multi-step approaches to three challenging small molecule targets. The same thinking enabled us to develop some new methods to engineer aptamers in a way that maximized conformational changes occurring near electrode surfaces leading to optimal receptors for electrochemical aptamer-based sensors (E-AB).

N-02-P**VARIANTS OF THE 3D COMPUTER MODEL
OF THE LiF-KF-RbF T-x-y DIAGRAM**V. Vorob'eva , A. Zelenaya , V. Lutsyk and M. Lamueva*Institute of Physical Materials Science (Siberian Branch of the Russian Academy of Sciences), 6
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Because of the many contradictions, connected with the literature data about the binary systems, which form the ternary LiF-KF-RbF one, three possible versions of the T-x-y diagram geometric structure of this system were proposed and their three-dimensional computer models had been designed.

N-03-P**THEORETICAL STUDY OF GEOMETRIES AND ENERGIES OF THE Pt...H INTERACTIONS**

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Geometries and energies of Pt...H interactions were studied using analysis of crystallographic data and quantum chemical calculations. Cambridge Structural Database (CSD) was searched for all crystal structures containing X-Pt...H-OH interactions. Analysis of geometrical parameters in crystal structures showed that in majority of crystal structures X-Pt...H interactions do not have tendency for linear arrangement. Based on the results of analysis of geometrical parameters, model systems for quantum chemical calculations were made. Results of quantum chemical calculations showed that in case of linear X-Pt...H arrangement (angle X-Pt-H = 180°) between PtS molecule and water calculated intermolecular interactions are repulsive, while in case of X-Pt...H interaction with the X-Pt-H angle value of 90° the interaction is attractive ($\Delta E = -2.42$ kcal/mol). These results of quantum chemical calculations are in good agreement with the results of the analysis of crystallographic data.

N-04-P**SYNERGISM IN THE EXTRACTION OF CATECHOL AND HYDROQUINONE FROM AQUEOUS SOLUTIONS BY THE DIETHYL ETHER/1-BUTANOL MIXTURES**

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Synergic effect in the extraction of catechol and hydroquinone from aqueous solutions by the diethyl ether/1-butanol solvent mixtures was investigated. Higher distribution ratios for both catechol and hydroquinone were obtained in the whole composition range of the diethyl ether/1-butanol binary mixture in comparison to extraction with pure solvents. For the same organic phases distribution ratios for catechol were higher than for hydroquinone, but the values of synergic coefficients were higher for hydroquinone.

O - Pharmaceutical Physical Chemistry

O-01-P

THE EFFECT OF NONIONIC BRIJ 35 MICELLES ON IONIZATION OF SIX ACE INHIBITORS

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The pK_a values of six ACE inhibitors (ACEI); captopril (Cp), cilazapril (Cz), enalapril (En), lisinopril (Ls), quinapril (Qp) and ramipril (Rp) have been potentiometrically determined in micellar solutions of Brij 35. Nonionic micelles affected the ionization of ACEI from -3.44 to +1.9 pK units in comparison to “pure” water. The change in distribution of equilibrium forms is significantly expressed at pH values of biopharmaceutical importance which may indicate on potential interactions with noncharged but polar molecules under the physiological conditions.

O-02-P

THE EFFECT OF NONIONIC SURFACTANTS ON IRBESARTAN AND LOSARTAN SOLUBILITY

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The solubility of two structurally similar sartans, irbesartan and losartan, were investigated at pH 4.5 (acetate buffer) in surfactant free media and in the presence of nonionic surfactants Brij 35 and TX-100 (10⁻³ mol/L). The solubility of both compounds is of the same order of magnitude in surfactant free media. The nonionic surfactants caused significant increase in losartan solubility (more than 100 times) but very slight increase in irbesartan solubility (only 2 times). The obtained results point out that imidazole moiety, where the main difference between chemical structures of examined sartans can be observed, could be responsible for interaction with the micelles of nonionic surfactants.

Q - Food Physical Chemistry

Q-01-P

ENERGY DISTRIBUTION BETWEEN MAIZE AND WEEDS

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The aim of the study was to investigate the variations in accumulation of dry substance and water in maize and weeds, induced by two herbicide types (applied pre- and post-emergence). Weeds tend to captivate higher energy amounts than crop plants. Greater free energy of water indicated increased energy consumption for non-spontaneous processes in weeds. Relatively unchanged net heat of combustion of maize and lower net heat of combustion of weeds indicated herbicide ability to reduce energy accumulation by weeds and to remain it constant in maize plants.

Q-02-P

**UHPLC-DAD-ESI-MS ANALYSIS OF THE ETHANOLIC
REISHI/PROPOLIS EXTRACT**

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Ultrahigh performance liquid chromatography coupled with diode array and mass spectrometry detectors (UHPLC-DAD-ESI-MS) was used for analyzing the composition of an ethanolic Reishi/Propolis extract (70:30 v/v). The extract contains a significant amount of polyphenols with the major contribution of flavonoids and phenolic acids, suggesting its potential role as an antimicrobial and antioxidant agent.

Q-03-P**LABORATORY SCALED EVALUATION OF SORPTION BEHAVIOR FOR FIVE PESTICIDES IN APPLE PEEL: EFFECT OF PESTICIDE CONCENTRATION**D. Anđelković¹, M. Branković² and G. Kocić³¹ *University of Niš, Agricultural Faculty, Kosančićeva 4, 37000 Kruševac, Serbia*² *University of Niš, Faculty of Sciences and Mathematics, Department of Chemistry, Višegradaska 33, 18000 Niš, Serbia (milica.chem@outlook.com)*³ *University of Niš, Faculty of Medicine, Bulevar dr Zorana Đinđića 81, 18108 Niš, Serbia*

Apples are frequently exposed to pesticides. Pesticide interaction with peel (cuticle and waxes) starts via absorption mechanisms. Sorption behavior affects the fate and persistence of the pesticides. This laboratory scaled study was designed to determine the residue levels of four fungicides and one insecticide in apple peel after fruit immersion in commercial pesticide solutions of several concentrations. The study showed that when increasing the pesticide concentration in solution, the in-peel amount of the fungicides and the insecticide increases exponentially and linearly, respectively.

Q-04-P**COMPOSITION OF BUCKWHEAT EXTRACTS DETERMINED BY UHPLC-LTQ OrbiTrap MS**M. Nešović¹, U. Gašić², N. Nedić³, S. Blagojević¹, Lj. Ignjatović⁴, Ž. Tešić⁵¹ *Institute of General and Physical Chemistry, Studentski trg 12-16/V, 11158 Belgrade, Serbia, (milicaffh@yahoo.com)*² *University of Belgrade, Department of Plant Physiology, Institute for Biological Research "Siniša Stanković", National Institute of Republic of Serbia, Bulevar despota Stefana 142, 11060 Belgrade, Serbia.*³ *University of Belgrade, Faculty of Agricultural Department, Nemanjina 6, 11080 Belgrade Zemun, Serbia.*⁴ *University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia.*⁵ *University of Belgrade, Faculty of Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia.*

Buckwheat is a high nutritional plant. It has great potential for the prevention of many diseases, mostly due to its antioxidant properties. As a functional food, it is recognized as a valuable plant for research. Ultra-high performance liquid chromatography coupled to linear trap quadrupole of a mass spectrometer and equipped with ion trap OrbiTrap (UHPLC-LTQ OrbiTrap MS) has been used to investigate the existence of polyphenols in buckwheat leaf, stem, flower and grain. It was shown that extracts of a different part of buckwheat, obtained by the solid phase extraction (SPE) method, possess a notable number of polyphenols. Prominent compounds were quercetin and its derivatives (rutin, quercitrin) and *p*-hydroxybenzoic acid. Compounds such as monomeric flavanol 3-ols (epicatechin

and its galloylated derivatives) and dimers (B type procyanidins) are identified in all four analyzed buckwheat samples, with dominant portion in buckwheat grain.

Q-05-P

RESEARCH OF QUALITY AND ANTIOXIDANT POTENTIAL OF HUMAN MILK AND INFANT FORMULA FOR LACTOSE-INTOLERANT INFANTS

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Infant food is a crucial component of development and normal growth of infants. Nutritive characteristics and methods for determination of the antioxidant potential of the infant food were compared in order to test the quality and biological value of human milk and infant formula with and without lactose. The antioxidant potential was determined using cyclic and differential pulse voltammetry, and electron paramagnetic resonance spectroscopy. Used electrochemical methods revealed high antioxidant potential of infant formula compared to human milk, while electron paramagnetic resonant spectroscopy revealed that the infant food possesses a significant capability to capture ·OH radicals and form carbon-centred radical in Fenton reaction. Lactose-free infant formula has high antioxidant potential and its application is important during diarrhea because infant food contributes to the reduction of pathogens by changing redox state of the environment in the infant's gastrointestinal tract.

Q-06-P**EXAMINATION OF PROOXIDATIVE ACTIVITY OF RED WINE IN MELANOMA CELLS**

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Melanoma is responsible for 75% of all deaths from skin cancer. Its lethality arises from its rapid progression, easy metastasis and drug-resistance as well. Red wine is a natural product rich in polyphenolic compounds with potent anticancer activities. It seems that in cancer cells these compounds behave as prooxidants initiating reactive oxygen species mediated cellular DNA breakage and consequent cell death. The aim of this study was to investigate prooxidative activity of red wine samples (Merlot variety, commercial as well as VCR1 and VCR101 clonal wines) in melanoma A375 cells, through measuring the relationship of reduced and oxidized form of glutathione (GSH/GSSG) and comparison with the GSH/GSSG ratio in control (untreated melanoma cells). The data obtained showed that tested red wine samples decrease GSH/GSSG ratio in A375 cells compared to control (4.6 ± 0), with the largest decrease noticed in treatment with VCR101 wine (0.66 ± 0.05).

R - Physico-Chemical Analysis

R-01-O**DETECTION AND ISOTOPIC DISTRIBUTION OF OXAPROZINE COMPLEX CONTAINING CU(II) IONS BY LDI MASS SPECTROMETRY**

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An oxa complex containing transition metal ions is potentially a great medication in anticancer therapies. In this work we used laser desorption/ionization (LDI) on a commercial matrix-assisted LDI time of flight mass spectrometry (MS) instrument to demonstrate possibilities for direct detection and obtainment of isotopic distribution of Oxaprozin metal complex with Cu(II) ions. Results show that the molecular ion of Oxaprozin metal complex with Cu(II) ions were detected at m/z 711.14, 712.13, 713.13, 714.13, 715.13, 716.10, at the range of laser intensity from 3300 to 3700 a.u., the accelerating voltage of 25000 V, the grid voltage of 60%, and the range extraction delay time from 100 to 300 ns. For the above mentioned instrumental parameters, the experimental isotopic distribution of Oxaprozin metal complex with Cu(II) ions is in a good agreement with its theoretical values. The LDI MS appears to be a promising method for characterization of new organometallic species.

R-02-O**ON POSSIBILITIES OF MINERAL PIGMENTS CHARACTERISATION USING LDI-MS: THE IRON-RICH EARTHY OCHER CASE**

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Earthy ochre sample originating from the Devil's Town, a rocky geological formation in the South Serbia region, was described using a laser desorption/ionization time-of-flight mass spectrometry (LDI-ToF-MS). Obtained laser desorption/ionization mass spectrum consisted dominantly of the series of chromium and iron (such as $\text{Fe}_{1-3}\text{O}_{1-3}$, $\text{Fe}_{1-2}(\text{OH})_{1-2}$, $\text{Fe}_{1-3}\text{O}(\text{OH})_{2-3}$, $\text{Cr}_{1-3}\text{O}_{2-9}$, $\text{Cr}(\text{OH})$, $\text{CrO}(\text{H}_2\text{O})$, $\text{CrO}(\text{OH})_4$, $\text{Cr}_2\text{O}_2(\text{OH})$). These oxides, hydroxides and oxyhydroxides species of chromium and iron indicates at presence Cr_2O_3 , CrO_3 , Fe_2O_3 and Fe_3O_4 in the sample.

R-03-P**DEVELOPING OF A METHOD FOR DETERMINING ASCORBIC ACID USING A SMARTPHONE AS A DETECTOR**

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The development of a method for the determination of ascorbic acid based on the reaction with Cu (II) -neocuproin using a smartphone is described. The absorbance of the reaction solution prepared from Cu (II) -neocuproin solution and standards / samples at a wavelength of 458 nm was measured spectrophotometrically. The solutions in the cuvettes were then imaged using a smartphone. The samples in the cuvettes were placed on a white background and photographed in daylight. During spectrophotometric and smartphone determination, ascorbic acid achieved a linear dynamic range of 2×10^{-5} - 1×10^{-3} mol L⁻¹. The analytical usability of the method was checked, using a spectrophotometer and a smartphone, in the analysis of real samples.

R-04-P**GC/MS PESTICIDES ANALYSIS IN APPLE PEEL: A METHOD FOR WAXES ELIMINATION**

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D

Apple peel as a natural barrier can retain some amount of applied pesticides and thus serve as an indicator of their presence. This study was conducted to establish a sample preparation method for GC/MS pesticide residue analysis in apple peel, which results in the elimination of waxes. The developed procedure is time- and cost-effective and does not implement the usage of sorbent or any other expensive consumables.

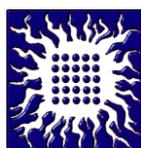
R-05-P**CHARACTERISATION 1,4-DISUBSTITUTED 2,5-DIKETOPIPERAZINES
BY ESI MASS SPECTROMETRY**

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The diketopiperazines have been steadily attracting researchers' attention in pharmaceutical chemistry due to their potential biological effects. Electrospray ionization mass spectrometry (ESI MS) is known to be a versatile analytical technique for detection of very low concentrations of various diketopiperazines in different samples. Hence, we characterized our p-disubstituted phenyldiketopiperazines **1** ($R = H$), **2** ($R = NO_2$) and **3** ($R = -N(CH_3)$) by ESI MS. We have shown that the majority of the fragment ions in the ESI mass spectra originated from reactions initiated by one of the nitrogen atoms of the piperazine ring.



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