CAS–ANSO CONFERENCE

Conference on Green Energy and Environmental Resilience

An International Forum for Sustainable Ecosystem Solutions

BOOK OF POSTER ABSTRACTS

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Poster Program

Poster Session 1 — Day 1 — Wednesday, 23 September

10:00 – 15:00 (continuous exhibition, ROMPHYSCHEM 18th edition & Networking Break)

Materials Sciences, Green Technologies and Sustainable Energy Conversion; Regional Initiatives for Environmental Preservation and Sustainability

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P3.09	Leonties, Anca Ruxandra	Salt Induced Activation of Trametes versicolor Laccase for Textile Dye Degradation
P3.10	Neacsu, Ana	Energy Valorization of Biomass Waste: Hydrothermal Carbonization of Orange Peels
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P3.21	Preda, Silviu	Calcium-Modified Titanate Nanotubes for Photocatalytic Processes
P3.22	Maxim, Catalin	Fine Structural Modulation Drives Circularly Polarized Luminescence in Helicoidal Zn(II) Coordination Polymers
P3.23	Musuc, Adina Magdalena	Effect of the Concentration of Hyaluronic Acid on the Pharmacotehnical Properties of Carbopol-Based Hydrogels
P3.24	Gîfu, Ioana Cătălina	Smart Microbial Polysaccharide Hydrogels for SustainableDecontamination of Antibiotic-Contaminated Waters
P3.25	Anastasescu, Mihai	Nano-Mechanical Assessment of Polyvinyl Alcohol Hydrogels Embedding Hafnia-Based Nanostructured Powders
P3.26	Predoană, Luminița	Ni and Ag Doped TiO_2 Nanopowders Prepared by the Sol-Gel Methodfor Stable Water-Based Nanofluids
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Poster Session 1

Day 1 — Wednesday, 23 September · 10:00 – 15:00 (continuous exhibition, ROMPHYSCHEM 18th edition& Networking Break)

Materials Sciences, Green Technologies and Sustainable Energy Conversion; Regional Initiatives for Environmental Preservation and Sustainability

P1.01 Silica-Based Materials for Photocatalytic Processes

Crina Anastasescu[1], Polona Umek[2], Veronica Bratan[1], Catalin Negrila[3], Silviu Preda[1], Catalina Gifu[4], Mihai Anastasescu[1], Maria Zaharescu[1], Ioan Balint[1]

1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependenţei, 060021 Bucharest, Romania
2.Jožef Stefan Institute, Jamova cesta 39, SI-1000 Ljubljana, Slovenia
3. National Institute of Materials Physics, 405A Atomiştilor, PO Box MG 7, 077125 Măgurele, Romania
4.National Research and Development Institute for Chemistry and Petrochemistry - ICECHIM, 202 SplaiulIndependentei, 060021 Bucharest, Romania

The development of novel engineered materials and their integration with renewable and clean energy sources, such as solar light have become imperative in current research. This work presents new approaches to the development of photoactive silica- based materials obtained by using the sol-gel method and various modifiers (compounds containing hafnium, copper, iron, and ruthenium). These were introduced to increase the density of optically active defects and promote the formation of new active interfaces. Reactive oxygen species (ROS) photogeneration and water splitting were investigated under simulated solar light irradiation (AM 1.5) and UV exposure. The morphological and structural properties of the materials were performed using scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), UV–Vis and photoluminescence (PL) spectroscopies, zeta potential measurements.

P1.02 Electrochemical Behavior of BiF_3-Based Electrodes in Liquid Electrolyte Systems for Fluoride Shuttle Batteries

*Pakpoom Athikaphan[1], Nicha Tabtimtong[2], Pattanapon Kaisook[2], Yumiko Imai[1], Tadashi Ueda[1], Arthit Neramittagapong[2], Sutasinee Neramittagapong[2], Taketoshi Minato[1,3]**

1. Institute for Molecular Science, National Institutes of Natural Sciences, 38 Nishigonaka, Myodaiji, Okazaki, Aichi, 444-8585, Japan
2. Department of Chemical Engineering, Faculty of Engineering, Khon Kaen University, Khon Kaen 40002, Thailand
3. Core for Spin Life Sciences, Okazaki Collaborative Platform, National Institutes of Natural Sciences, Okazaki, Aichi 444-8585, Japan
Corresponding author: minato@ims.ac.jp

Fluoride shuttle batteries (FSBs) are promising candidates for next-generation energy storage owing to their high theoretical energy density based on reversible metal fluoride conversion reactions. However, the practical development of liquid-electrolyte FSBs remains limited by insufficient fluoride availability and sluggish electrode kinetics. In this study, $NaBF_4$- and KPF_6-based electrolytes were preliminarily evaluated for their ability to enable reversible electrochemical reactions in a BiF_3-based electrode system. Galvanostatic charge–discharge measurements showed reversible cycling behavior during the first three cycles. The electrode delivered discharge capacities of approximately 270 mAh g^{-1}, with corresponding charge capacities of around 120–195 mAh g^{-1}. The voltage profiles exhibited distinct discharge and charge regions, indicating that the KPF_6-containing electrolyte may facilitate fluoride transfer and partially sustain the BiF_3/Bi conversion reaction. Although capacity fading was observed upon cycling, these preliminary results demonstrate the potential feasibility of this electrolyte system for fluoride-based electrochemical energy storage.

Overall, these preliminary findings indicate that KPF_6 is a promising electrolyte component for liquid-electrolyte fluoride shuttle batteries. This work provides an initial basis for further investigation into electrolyte design, reaction mechanism, and interfacial stabilization for improved reversible fluoride storage.

P1.03 Balsa Wood Modification Using a Microwave-Assisted Boron–Silica–CuO Fire-Retardant System

Mariana Patrascu[1,2], Simona Petrescu[3], Gabriela Marinescu[3], Silviu Preda[3], Raul Augustin Mitran[3], Daniel Lincu[3], Soare Elena Mirabela[3], Ana Maria Seciu-Grama[4], Jeanina Pandele Cusu[3], Irina Atkinson[3]**

1.National University of Science and Technology Politehnica of Bucharest, 313, SplaiulIndependenței, 060042 Bucharest, Romania,
2.Safety Integrated Solutions S.R.L., 33, Cătănoaia, 032903 Bucharest, Romania
3."Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
4.National Institute of Research and Development for Biological Sciences, 296SplaiulIndependentei, 060031 Bucharest, Romania
Corresponding authors: iatkinson@icf.ro, jeanina@icf.ro

Balsa wood is widely used in a variety of applications owing to its exceptionally low density. However, its high flammability limits its use in applications requiring enhanced fire safety. This study aimed to develop a boron–silica-

based fire-retardant system incorporating biosynthesized copper oxide nanoparticles (CuO NPs) at concentrations of 1 and 3 wt% via a microwave-assisted method. The resulting fire-retardant system was applied to balsa wood by immersion. The treated wood was characterized using scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDX), Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and thermogravimetric/differential thermal analysis (TG/DTA).
SEM–EDX analysis confirmed the uniform deposition of the fire-retardant on the balsa wood surface and the successful incorporation of CuO NPs. TG/DTA results demonstrated improved thermal stability and increased char formation compared with untreated balsa wood. Fire-retardant performance was evaluated using the Vertical Flame Test (VFT). The VFT results demonstrated reduced flame propagation and enhanced self-extinguishing behavior, indicating a synergistic effect between the boron–silica matrix and CuO NPs. Furthermore, fire-retardants containing CuO NPs exhibited effective antibacterial activity against Staphylococcus aureus. Overall, the boron–silica–CuO fire retardant system represents a sustainable and multifunctional strategy for improving the fire resistance and antibacterial performance of balsa wood.

Acknowledgements
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P1.04 Nd-Fe Alloys Obtained by an Electrochemical Process of the Oxides in Chloride Molten Media

*V.Soare[1], M.Burada[1], M.Tarcolea[2], A.M.Popescu[3], V.Constantin[3]**
1.National Research-Development Institute for Nonferrous and Rare Metals-IMNR, 102 Biruinţei B-lvd, Pantelimon, 077145Ilfov, Romania
2.POLITEHNICA University of Bucharest, Biomaterials Research Centre-BIOMAT, 313 SplaiulIndependenţei, 060032Bucharest, Romania
3.“Ilie Murgulescu” Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania, Laboratory of Molten Salts, 202SplaiulIndependentei, 006021Bucharest, Romania

With their excellent magnetic characteristics, abundant raw materials and relatively low prices, the permanent magnets based on Nd-Fe alloys are classical produced via molten salt electrolysis or metallothermic reduction using fused fluoride-chloride or fluoride-oxide media. In the present paper, the experimental results for the Nd-Fe alloys obtained by electrochemical reduction of a pressed and sintered mixture of Nd_2O_3 and Fe_2O_3. The electrolyte is molten calcium chloride. Obtaining Nd-Fe alloy directly from oxides dissolved in molten $CaCl_2$ is achieved by electrolysis in molten salts. This method is an ecological and cheaper alternative to traditional processes that use toxic fluorides.

P1.05 Thermocatalytic Ammonia Synthesis over LDH Derived Mixed Oxides Supported Ru/Rh Nanoparticles

Liubovi Cretu[1], Razvan State[1], Monica Pavel[1], Mihai Alexandru Cristea[2], Ioan-Cezar Marcu[3], Ioan Balint[1], Florica Papa[1]
1. “Ilie Murgulescu” Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania;
2. University of Bucharest, Faculty of Biology, 91-95 SplaiulIndependenţei, Bucharest, Romania;
3. University of Bucharest, Faculty of Chemistry, 4-12, Bulevardul Regina Elisabeta, 030018 Bucharest, Romania

Mixed oxide supports derived from LDH precursors (CoMgAlO and CoAlO) were synthesized by controlled coprecipitation at 60 °C and pH 10, followed by maturation, washing to neutrality, drying at 80 °C, and calcination at 700 °C for 8 h. Mono and bimetallic Ru, Rh, and Ru–Rh nanoparticles were prepared via the polyol method using ethylene glycol, PVP, and alkaline conditions, with optional Cs^+ promotion. Nanoparticles were deposited either by impregnation or by synthesis in the presence of the support, enabling controlled assembly and dispersion.
The influence of synthesis parameters including support composition, promoter concentration, and nanoparticle structure on morphology and surface properties was examined. Reducibility was assessed by H_2-TPR, revealing distinct Co^{2+}/Co^0 and Co^{3+}/Co^{2+} transitions and temperature dependent metal–support interactions. CO_2 desorption and H_2 chemisorption provided insight into basicity and metal dispersion, while TEM confirmed nanoparticle morphology. LDH derived CoMgAlO calcined at 600 °C retained higher catalytic activity than the 700 °C analogue.
Catalytic performance in ammonia synthesis at 10 atm was evaluated using a continuous flow system equipped with mass flow controllers, temperature control, back pressure regulation. Rh/CoMgAlO_600 consistently outperformed Rh/CoMgAlO_700 across 350–650 °C. CoAlO(LDH) and CoMgAlO(LDH) alone exhibited negligible activity, confirming the necessity of supported Rh. The Ru–Cs/CoMgAlO catalyst displayed enhanced activity due to Cs induced electronic promotion, while Rh/CoMg O (mixed oxide) and Rh–Cs/CoMg O (mixed oxide) highlighted the influence of support origin (LDH vs. non LDH) and promoter addition. Ammonia formation was quantified by conductivity measurements of H_2SO_4 solution neutralization.
Overall, the results offer design principles for creating more effective Ru and Rh based catalysts for ammonia synthesis under milder operating conditions.

P1.06 SnO_2-ZnO-Fe_2O_3 Multicomponent Thin Films for Propane Sensing Applications

Izabella Dascalu, Mirela Enache, Jose Maria Calderon Moreno, Veronica Bratan, Cristian Hornoiu, Simona Somacescu
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

Metal oxide thin films represent promising materials for gas sensing applications due to their tunable physicochemical properties and their ability to respond to different target gases. The design of multicomponent oxide systems represents an effective strategy for tailoring the structural, surface, and functional characteristics required for the development of advanced sensing materials. This work focuses on the preparation of SnO_2–ZnO–Fe_2O_3 multicomponent thin films by the sol-gel spin-coating technique and the investigation of their properties for propane sensing applications. Characterization of the obtained films confirmed the successful formation of SnO_2–ZnO–Fe_2O_3 multicomponent thin films and revealed that the incorporation of Zn and Fe into the SnO_2 matrix modifies the structural, optical and electrical properties of the material. These changes were found to influence the sensing performance toward propane, with the lower Fe-containing composition exhibiting the highest response, which was attributed to its favorable surface morphology and enhanced active surface area. The correlation between composition, material properties and gas sensing behavior highlights the potential of SnO_2–ZnO–Fe_2O_3 multicomponent thin films as promising candidates for propane detection and environmental gas monitoring applications.

P1.07 Properties of Metal-Organic Frameworks Based on Terephthalic Acid

M. Boșomoiu[1], A. Dinu[1], A. C. Stănicel[1], G.C. Roșianu[1], F. Papa[2],M. Deaconu[1,3], C. Matei[1], D. Berger[1]**
1.Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 1-7 Polizu Street, 011061 Bucharest, Romania
2."Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
3.CAMPUS Research Institute, National University of Science and Technology Politehnica Bucharest, 313 SplaiulIndependentei, 060042 Bucharest, Romania
Corresponding authors: anton.dinu@stud.chimie.upb.ro, daniela.berger@upb.ro

Metal-organic frameworks (MOFs) consist of nanosized metal-oxide clusters, separated by organic linkers, arranged in a crystalline lattice having a micropore framework. Recently, research interest in MOFs has increased due to their versatile structure, depending on the synthesis conditions, very high porosity and uniform micropore network, acidic properties that can be modulated by doping or through organic groups functionalization. Based on their good adsorption properties, MOFs have been studied for various applications such as energy storage [1], environmental remediation [2], separation, catalysis, drug delivery [3] etc.
This study deals with obtaining and characterization of MOFs based on terephthalic acid derivatives, UIO-66(Zr), UIO-66-NH2(Zr) and MIL-53(Al). MOF samples were characterized by X-ray diffraction, FTIR spectroscopy, thermal analysis, and scanning electron microscopy. The N_2 adsorption-desorption isotherms recorded at 77 K for all synthesized MOFs were type I specific for microporous materials, and high specific surface area were obtained, the values being in the range of 926-1340 m^2/g. The micropore distribution curves were determined based on CO_2 adsorption isotherms recorded at 273 K. The adsorption properties of synthesized MOFs were investigated using aqueous solution of Alizarin red. The adsorption kinetics of the dye was also investigated using an aqueous solution with a concentration of 150 mg/L. The highest adsorption capacity was observed for the UiO-66 sample.

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P1.08 Surface Fractal Analysis as a Complementary Tool for Characterizing LDH-Derived Mixed Metal Oxide Catalysts

Gianina Dobrescu, Florica Papa, Liubovi Cretu, Ioan-Cezar Marcu, Ioan Balint
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

Layered double hydroxides (LDHs) based on Mg-Al, Ca-Al, and their Cu-containingforms were prepared by co-precipitation, with careful adjustment of the composition andratios of the metal precursors to produce 10g of Mg 2 AlO 3.5, Ca 2 AlO 3.5, and the Cu-containing Cu 0.45 Mg 1.55 AlO 3.5, Cu 0.45 Ca 1.55 AlO 3.5 mixed metal oxides. X-ray diffraction, nitrogen adsorption-desorption, and surface fractal analysis applying both the fractal adsorption isotherm model and a thermodynamic method were used to characterize the LDHs.

It was noted that the highest specific surface area is showed by MgAlO (145.58 $m^2 \cdot g^{-1}$), meanwhile introduction of 15 at% Cu reduced both surface area and microporosity,increasing the average pore diameter to 11.4 nm.
Adding copper had a different impact on the textural characteristics of the Ca-Al mixedoxides leading to higher BET surface areas.Fractal analysis showed that the surface fractal dimensions varied, with CaAlO havingrelatively smoothand homogeneous surface with very little porosity and MgAlOdisplaying highly heterogeneous hierarchical structures.
The fractal dimensions obtained using the thermodynamic approach are in goodagreement with those obtained from the fractal adsorption isotherm model, supportingthe consistency between the two methods. The Cu-containing mixed oxides were testedas catalysts in the hydrodeoxygenation of benzyl alcohol. Their catalytic activity wasfound to be linked to their surface texture and morphology, showing that fractal analysisadds to standard textural characterization and helps clarify the connection between porestructure and catalytic behavior.

P1.09 A Straightforward Route to Prepare MoO_3-$K_2Mo_8O_{13}$ Heterostructures: in the Search of New Materials for Electrochemical Energy Storage Devices

Cristina Donath[1], Diana Visinescu[1], Maria-Gabriela Alexandru[2],Adelina – Carmen Ianculescu[3], Loredana Preda[1], Elena Ionela Neacsu[1], Tanta Spataru[1]

1. "Ilie Murgulescu"Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2.Department of Inorganic Chemistry, Physical Chemistry and Electrochemistry, Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 1-7 Gh. Polizu Street, 011061 Bucharest, Romania
3.Department of Science and Engineering of Oxide Materials and Nanomaterials, National University of Science and Technology Politehnica Bucharest, Bucharest, 060042, Romania

Molybdenum-based oxides or hybrid structures, with 1D morphologies (wires, fibers, rods, orbelts), were attractive for electrochemical applications due to the large electrode–electrolyte contact area, facile strain relaxation and efficient 1D electron transport pathway. For example, the bi-layered structure of α-MoO_3 can host Li^+, Na^+ or K^+ cations, which makes it a suitable electrode for Li/Na/K-ion batteries or for charge storage applications [1]. Herein we report on rare examples of K/Mo oxide materials hybrid structures, with 1D morphologies, of which capacitive properties and their potential in energy storage applications were explored. Micro-sized ribbon- and belt-like materials were obtained via a single molecular precursor approach, through hydro-/solvothermal synthesis, by employing potassium octacyanomolybdate complex, and subsequent calcination treatments. The composition, crystallinity and morphologies of the as-obtained materials were investigated through XRD and SEM/TEM/HR-TEM methods [2]. The molybdenum oxides-modified electrodes showed good capacitive properties (12.65 F/g at a sweep rate of 20 mV s^{-1}) in cyclic voltammetry (CV) as well as in galvanostatic charge discharge (GCD) tests. The crystallinity, composition and morphology of K/Mo oxide materials play key roles in their electrochemical performance. To improve the charge storage capacity, we carried out electrochemical investigations on the electrode modified with a mixture of K/Mo oxides and conductive graphene or porous carbonaceous materials derived from natural carbohydrates. Our results open a large perspective in the design of new generation of highly efficient capacitors with modulated compositions and tailored morpho-structural features.

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P1.10 Physicochemical Investigation of Intermolecular Interactions using Volumetric, Ultrasonic and Optical Techniques, for 1-chlorohexane + Aromatic HydrocarbonsBinary Mixtures

Dana Drăgoescu*,Florinela Sîrbu*

"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, SplaiulIndependentei202, 060021 Bucharest, Romania
Corresponding authors: ddragoescu@icf.ro,sflorinela@yahoo.com

The physico-chemical properties for two binary mixtures of 1-chlorohexane with some aromatic hydrocarbons, as n-propylbenzene and iso-propylbenzene, were measured. The data for densities, speeds of sound, and refractive indices, are obtained at several temperatures in the range of (293.15 to 318.15) K and p = 0.1 MPa. By using the experimental results, the excess molar volumes, the partial/apparent molar volumes, the isentropic compressibilities, the excess molar isentropic compressibilities, as well as the deviation in refractive indices, and the excess molar refractions were calculated and reported at T = 298.15 K in this work.
All the deviation and excess properties have been correlated with the Redlich-Kister polynomial equation.
Discussions concerning the experimental and calculated results in relation to the molecular interactions and structural effects between components of mixtures are presented.

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P1.11 Corrosion Behavior of Inconel 718 Alloy Processed by SLM after 5000 Hours of Exposure to Natural Seawater (Red Sea)

*E.I. Neacsu[1], F. Branzoi[1], M. Anastasescu[1], A. Banu[1], A. Paraschiv[1], A. Bibis[1], M. Marcu[1]**
1."Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, Bucharest, Romania
2.Romanian Research and Development Institute for Gas Turbines COMOTI, Iuliu Maniu 220D, 061126 Bucharest, Romania
3.Surface Engineering and Corrosion Laboratory, Faculty of Industrial Engineering and Robotics, National University of Science and Technology Politehnica Bucharest, 313Splaiul Independentei,060042 Bucharest, Romania
Corresponding author: m_marcu@icf.ro

The corrosion behavior of Inconel 718 produced by conventional forging (S1) and selective laser melting (S2) was systematically studied in natural seawater. Electrochemical characterization was performed at room temperature during long-term immersion in natural seawater (Red Sea) using potentiodynamic polarization measurements to evaluate the corrosion resistance and stability of the passive film. Morphological analysis of the alloy's surface, performed using scanning electron microscopy (SEM) coupled with energy dispersive X-ray spectroscopy (EDS), revealed a continuous, compact film with localized salt deposits on both alloys. The morphology of the samples, analysed by AFM, appears to have changed after the corrosion experiments. The roughness histograms indicate an abrupt increase in surface corrugation (S1 > S2). After 5000 hours of immersion, the corrosion parameters obtained from Tafel curves indicate that the SLM 718 alloy (S2) exhibits good corrosion resistance (Rcorr = 35 µm y^{-1}). This high resistance is attributed to the development of a thicker and more stable surface film, which further improves corrosion resistance. Notably, surface analysis of both samples after 5000 h of immersion indicated no localized corrosion, confirming the alloys' resistance to marine corrosion

P1.12 Influence of the Composition and Substrate on the Properties of the Perovskite Films

M.Gartner[1], M. Anastasescu[1], J. Calderon-Moreno[1], S. Preda[1], I. Atkinson[1], H. Stroescu[1],M. Nicolescu[1], M.Chelu[1], D. Mitrea[1], E. Radeva[2], M. Ganchev[2], V. Palankovski[2], S. Spasova[2], S. Topalski[2]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy,202 SplaiulIndependentei, 060021, Bucharest, Romania
2. Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences,72 TzarigradskoShaussee Blvd., 1784 Sofia, Bulgaria

Copper–tin sulfide and tin sulfide thin films were deposited by chemical bath deposition on TiO_2/glass and ITO/glass substrates in order to investigate the influence of composition and substrate nature on their structural, morphological and optical properties for photovoltaic applications. Films containing Cu/Sn ratios of 1:1 and 2:1, together with SnS layers, were synthesized under identical deposition conditions and characterized by X-ray fluorescence (XRF), grazing incidence X-ray diffraction (GIXRD), atomic force microscopy (AFM), Raman spectroscopy, spectroscopic ellipsometry and optical transmission measurements.
XRF analysis confirmed the incorporation of Cu and Sn in the deposited layers, while XRD revealed that Cu–Sn films deposited on TiO_2 are predominantly amorphous, whereas SnS films deposited on ITO exhibit a crystalline orthorhombic phase accompanied by diffraction features originating from the ITO substrate. AFM investigations showed a strong dependence of surface morphology on film composition, with RMS roughness values ranging from 46.0 nm for Cu/Sn (1:1) films to 120.5 nm for Cu/Sn (2:1) layers, while SnS films displayed cauliflower-like or granular morphologies depending on the substrate. Optical measurements evidenced high absorption coefficients reaching values close to 4×10^4 cm^{-1} in the visible region, making these materials attractive candidates for photovoltaic applications. The Cu/Sn (1:1) film exhibited the highest optical transmission at 630 nm (64.9%), whereas the Cu/Sn (2:1) sample showed the largest absorption coefficient. The optical band gap decreased from 2.34 eV to 2.24 eV with increasing Cu content. Raman spectroscopy confirmed the presence of characteristic vibrational modes associated with Sn–S and copper sulfide phases.
The obtained results demonstrate that both the film composition and the substrate significantly influence the crystallinity, morphology and optical response of chalcogenide thin films, highlighting their potential as absorber materials for hybrid perovskite solar cell architectures.

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P1.13 Magnesium Oxide Synthesized through Precursor Method and its Application as Photocatalyst

D. Gingașu, G. Petcu, D.C. Culiță, J. Pandele-Cușu, L. Predoană, S. Petrescu, S. Preda
"Ilie Murgulescu" Institute of Physical Chemistry, 202 SplaiulIndependentei, 060021 Bucharest, Romania

For many years, researchers have focused their efforts on the preparation of metal oxides with wide applications in the industrial and technological domains. A special attention was given to magnesium oxide (MgO), due to its unique chemical, optical, mechanical, and electrical properties. These properties, along with its low cost and non-toxicity, have led to the use of magnesium oxide in different applications, such as: optical coatings, sensors, antimicrobial agent, water treatment, catalysis, and adsorbents. To the preparation of MgO, various methods have been proposed such as: sol-gel method, solid-state reaction, hydrothermal synthesis, and combustion process.
In this work, MgO nanoparticles were synthesized by precursor (thermal decomposition of coordination compounds) method, using tartaric and gluconic acids as ligands. Two types of complex precursors of MgO were isolated and were characterized by elemental chemical analysis, FT-IR spectra and thermal analysis. The structural, morphological, textural and optical properties of MgO were investigated by XRD, FT-IR and UV-Vis spectroscopy, SEM and nitrogen adsorption – desorption analysis. The obtained materials were tested in photocatalytic degradation of methyl orange dye under ultraviolet and visible light irradiation.

P1.14 Deflagration Parameters of Ethane-Air Mixtures

Venera Giurcan[1], Elena-Cristina Traneci[2], Diana Iuliana Preda[2], Tudor Tutui[3], Maria Mitu[1], Codina Movileanu[1]
1."Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania
2. Faculty of Mechanical Engineering and Mechatronics, National University of Science and Technology POLITEHNICA Bucharest, Romania
3. "Ion Neculce" National College, Bucharest, Romania

Ethane is a highly flammable gas used as a feedstock in the chemical industry and as a fuel or refrigerant in specialized industrial installations. The study of ethane-air mixtures is essential for improving industrial safety, limiting accidental pollutant emissions, and protecting personnel involved in the handling, use, and transport of combustible gases. A detailed characterization of their combustion and explosion behavior is required for preventing accidents and designing effective explosion-protection systems. The present study investigates the propagation parameters of deflagrations in stoichiometric ethane-air mixtures occurring in closed vessels obtained by both measurements and calculations. The maximum explosion pressure, deflagration severity factor, maximum rate of pressure rise, laminar burning velocity, and adiabatic flame temperatures under constant-pressure and constant-volume conditions were evaluated, together with their dependence on the initial pressure and temperature. The results showed that increasing the initial pressure increased the maximum explosion pressure, severity factor, and maximum rate of pressure rise, while decreasing the laminar burning velocity and adiabatic flame temperatures, whereas increasing the initial temperature enhanced the laminar burning velocity but reduced the maximum explosion pressure, severity factor, and maximum rate of pressure rise, with the corresponding effects on the adiabatic flame temperatures depending on the thermodynamic constraint considered. The findings contribute to a better understanding of ethane combustion and provide useful information for evaluating explosion hazards and designing protection systems for industrial installations involving combustible gases.

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P1.15 Hydrothermal Synthesis of High Entropy Perovskite Oxide Materials Synthesis for Energy Applications

M.C. Licu[1], F. Maxim[1], F. Teodorescu[1], D. Berger[2], I. Atkinson[1], S. Tanasescu[1]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy
2. Faculty of Chemical Engineering and Biotechnology, Polytechnic University of Bucharest

As the use of renewable and alternative energy sources increases, there is a growing need for materials that can store energy efficiently and reliably. High entropy perovskite oxides (HEPOs) have attracted significant attention due to their enhanced ferroelectric relaxor behavior, which directly underpins their energy storage performance. This concept relies on high configurational entropy, which promotes the formation of a single-phase perovskite structure with

intrinsic cationic disorder and local lattice distortion — the structural origin of the relaxor ferroelectric response [1]. Among the various synthesis routes, hydrothermal synthesis offers a low-temperature, single-step alternative to conventional solid-state reaction, which typically requires high calcination temperatures [2]. By promoting homogeneous mixing of multiple cationic species at the atomic level within an aqueous medium, this method facilitates the uniform cationic distribution needed for single-phase HEPO formation, while also offering finer control over crystallite size, morphology and stoichiometry, all without the risk of cation volatilization associated with high-temperature routes.
In this work, titanate based HEPO powders were synthesized via a hydrothermal method at 200 °C and 1000 rpm for 4 h, the resulting phases being characterized by X-ray diffraction (XRD). The XRD patterns confirmed the formation of single-phase perovskite structure with cubic or tetragonal symmetry and small crystallite sizes. These results support the hydrothermal route as a promising strategy for producing phase-pure HEPOs for energy storage applications.

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P1.16 Mesoporous Silica - KNO_3 Composite Phase Change Materials for Thermal Energy Storage

Daniel Lincu[1], Simona Ioniță[1], Cristian Matei[2], Daniela Berger[2], Raul-Augustin Mitran[1]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependenței, 060021 Bucharest, Romania
2. National University of Science and Technology “Politehnica” Bucharest, Faculty of Chemical Engineering and Biotechnologies, 1-7 Polizu Street, 011061, Bucharest, Romania

Molten nitrate salts confined within porous matrices have emerged as promising composite phase change materials (PCMs) for thermal energy storage (TES), offering the potential to combine the high energy-storage capacity of inorganic salts with the structural stability and tunable porosity of mesoporous hosts [1]. In this context, modification of the silica framework represents a promising strategy for tailoring the interaction between the porous matrix and the confined salt, with potential consequences for salt loading, phase transitions, and thermal storage performance [2, 3].
The present study investigates the influence of doping of mesoporous silica matrices designed as hosts for molten KNO_3-based composite PCMs. Mesoporous silica materials with different metal dopants were synthesized and systematically characterized to evaluate the effects of framework modification on their structural and compositional properties. The doped silica matrices were subsequently loaded with KNO_3 to obtain composite PCM systems. The relationship between the characteristics of the porous hosts and the amount and distribution of incorporated salt was investigated, together with the effects of confinement on the thermal behavior of KNO_3. Structural and thermal characterization was employed to assess changes in phase-transition characteristics, thermal stability, and the interaction between the nitrate phase and the modified silica framework.

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P1.17 Preliminary Spectroscopic Study of Eco-Friendly Compounds

*Carla-Cezarina Pădureț, Ana-Maria Manea-Saghin**
Research Center for Environmental Protection and Eco-Friendly Technologies, National University of Science and Technology POLITEHNICA of Bucharest, 1–7 Polizu Street, 011061 Bucharest, Romania
Corresponding author: am_manea@yahoo.com

Organic compounds have been extensively studied in the past decades due to the presence of conjugated systems with π-electrons which allows them to be widely employed for the manufacture of electronic and optoelectronic devices. Eco-friendly materials are preferred as alternative to synthetic compounds since they also exhibit outstanding optical properties [1,2]. In this regard, we have used in this study various natural-origin extracts such as blackberry, raspberry and black elderberry. The characterization of optical properties was realized using UV-Vis, fluorescence spectroscopies, while GC-MS analysis has been employed for the quantification of main bioactive compounds. Evaluation of the linear optical properties via UV-Vis analysis has shown an absorption band around 230 nm due to the presence of aromatic rings from polyphenols and flavonoids, while the fluorescence analysis contributed to identify

the main peaks assigned to emission and excitation processes. The Stokes difference has shown that the studied materials could be successfully used to prevent self-absorption of the emitted light in devices as OLED or QLED.

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P1.18 Laminar Burning Velocities of Inert-Diluted Propane-N_2O Flames

Maria Mitu[1], Venera Giurcan[1], Codina Movileanu[1], Domnina Razus[1], András György Szanthoffer[2]*, Siyabonga Nxumalo[2], Tamás Turányi[2]*
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania
2. Institute of Chemistry, Eötvös Loránd University, Budapest, Hungary
Corresponding authors: maria_mitu@icf.ro,andras.gyorgy.szanthoffer@ttk.elte.hu

The flammability behavior of propane-N_2O-inert gas mixtures is of considerable interest for assessing explosion hazards and developing effective safety strategies in industrial applications. Nitrous oxide is an attractive oxidizer because of its stability under ambient conditions and its compatibility with commonly used engineering materials. In this study, flame propagation in propane-nitrous oxide-inert (inerts: helium, argon, nitrogen, carbon dioxide) gas mixtures with various initial pressures (0.5–1.75 bar) and compositions was investigated using pressure-time records obtained in a spherical vessel with central ignition. Laminar burning velocities were determined from experimental pressure–time measurements during the incipient stage of closed-vessel explosions. The experimental burning velocities were compared with values predicted by combustion kinetic mechanisms from simulations of freely propagating premixed laminar flames. Simulations were performed using Cantera, accounting for multicomponent transport, the Soret effect, and radiative heat transfer. The following five chemical kinetic mechanisms were used: Aramco-2016_C3+ELTE_C1-NOx (combination of the C0-C3 chemistry of the Aramco-2016 mechanism [1] and the NOx and C1-NOx chemistry from Kovács et al. [2]); C3MechCoreV4.0.1 [3]; Ge-2026 [4]; POLIMI_C1_C3_HT_NOX [5]; and the C0-C3+NOx chemistry from the C3MechV4.0.1 detailed mechanism [6]. The results show that all investigated mechanisms tend to significantly underestimate the measured laminar burning velocities. The baric coefficients of laminar burning velocities and overall reaction orders of propane oxidation with nitrous oxide were determined.

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P1.19 Hydrogen Influence on Ignition of Multifuel – Air Deflagration

Codina Movileanu, Venera Giurcan, Maria Mitu
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania
Corresponding author: cmovileanu@icf.ro

The hydrocarbon-air combustion can be improved by adding small quantities of hydrogen. The method is beneficial as it provides a more stable combustion, especially in confined conditions and determines the decrease of hydrogen burning velocity, decreasing thus its reactivity and allowing for safer working conditions. The influence of adding of various amounts of hydrogen on the ignition by electric sparks of stoichiometric LPG-air mixtures was investigated at ambient initial temperature and various total initial pressures between 0.3 and 1.0 bar. The flanged electrode technique using high voltage inductive-capacitive sparks was used to measure the quenching distances, dq. for fuel-hydrogen-air mixtures. The total initial pressure p_0 and concentration of added hydrogen were found to influence this parameter. At constant composition, the quenching distances decrease with increasing pressure according to the following empirical correlation: $dq=a \bullet p_0^{-\alpha}$, where a is a constant and α is the baric coefficient.
The overall kinetic parameters of H_2-blended LPG oxidation were calculated as: the overall reaction order n from the baric coefficient of quenching distances ($n=-2 \bullet \alpha$) and the overall activation energy E_a from the variation of quenching distances versus the reciprocal value of average temperature of the flame front. Minimum ignition energies for ignition by high voltage sparks, H_{min} were calculated from the quenching distances according to a validated correlation model: $H_{min}=k \bullet p_0 \bullet dq^3$, where k is a proportionality constant and p_0 - the total initial pressure of mixture. All parameters were examined in correlation to the added hydrogen amount to LPG-air mixtures. The maximum experimental safe gap (MESG) was also calculated for the investigated mixtures and analysed in concordance with the total initial composition and concentration of added hydrogen.

P1.20 Testing of Ammonia/Methanol Combustion Mechanisms

Siyabonga Nxumalo[1], András Szanthoffer[1], Máté Papp[1], Tibor Nagy[1], Boyang Su[2], Tamás Turányi[1]
1. Eötvös Loránd University Institute of Chemistry
2. Chinese Academy of Sciences Institute of Engineering Thermo-physics

Ammonia (NH_3) is a promising carbon-free energy carrier, but its practical application as a fuel is limited by its low reactivity, high autoignition temperature, and low flame propagation speed. Blending ammonia with more reactive fuels is a potential strategy for improving its combustion characteristics. Methanol (CH_3OH) is particularly attractive because of its high reactivity, potential renewable production, and favourable storage and handling properties.
This work aims to quantitatively evaluate detailed NH_3/CH_3OH combustion mechanisms using a comprehensive collection of experimental data and improved estimates of experimental uncertainty. More than 4000 experimental data points have been collected from 15 peer-reviewed publications, covering temperatures of 650–2000 K, pressures of 1–49 atm, and equivalence ratios between 0.1 and 2.0. The database includes ignition delay times measured in shock tubes and rapid compression machines, laminar burning velocities, and species concentration profiles measured in jet-stirred and flow reactors. The experimental data are processed and encoded in ReSpecTh Kinetic Data (RKD) XML format [1-3] for standardised simulation and mechanism evaluation.
Particular attention is given to experimental uncertainty, which directly influences the quantitative assessment and subsequent optimisation of kinetic mechanisms. The Minimal Spline Fit method is applied to estimate the statistical noise of experimental data series by fitting polynomials and Akima splines of increasing flexibility and identifying a noise-free underlying trend without overfitting the experimental scatter. The statistical uncertainty estimated from the optimal fit is combined with the reported experimental uncertainty to obtain more representative standard deviations for mechanism evaluation.
Detailed kinetic mechanisms are tested using the in-house developed Optima++ framework [4], with their performance quantified using an error function that accounts for the estimated experimental uncertainties. Preliminary mechanism testing is used together with the Minimal Spline Fit analysis in an iterative procedure to identify datasets requiring further uncertainty refinement and to improve the statistical reliability of the experimental database.
The resulting uncertainty-refined database provides a robust basis for comprehensive mechanism comparison, sensitivity analysis, and future optimisation of important kinetic and thermochemical parameters. Ultimately, this work contributes toward the development of a more accurate and reliable kinetic mechanism for predicting NH_3/CH_3OH combustion over a wide range of operating conditions.

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P1.21 Combustion Experimental Data, Reaction Mechanisms, and Computer Codesfor Model Analysis and Development in the ReSpecTh Information System

Tamás Turányi[1], István Gy. Zsély[1], Máté Papp[1], Tibor Nagy[2]
1. Institute of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary
2. HUN-REN Research Centre for Natural Sciences, Budapest, Hungary

The ReSpecTh Information System [1] was created in 2014 as a joint website [2] for publishing datasets, models, and utility codes in the fields of gas-phase reaction kinetics (Re), high-resolution molecular spectroscopy (Spec), and thermochemistry (Th). The datasets contain validated experimental, empirical, and computed, machine-searchable data, and the corresponding metadata. The reaction kinetics (Re) branch contains directly measured and theoretically calculated rate coefficients, as well as indirect experimental data (ignition delay times, laminar burning velocities, and concentrations measured in flow reactors, jet-stirred reactors, micro-reactors, and flames). These data are stored in ReSpecTh Kinetics Data (RKD) format files [3]. The amount of published data continuously increases and now includes a large number of indirect (252,582 data points in 5,538 RKD data files) and direct (9,092 data points in 470 RKD data files) values. These data are related to the combustion of hydrogen, syngas, methanol, ethanol, methane, ethylene, $H_2/O_2/NO_x$, syngas/NO_x, methanol/NO_x, ammonia, butanol, C5-C12 alkanes and dimethyl carbonate. Several hundred published detailed reaction mechanisms in CHEMKIN format are provided for these combustion processes. The published utility codes include Optima++ [4] (creation and utilization of RKD format files; framework code for simulations using simulation codes Cantera, OpenSMOKE++, FlameMaster and Zero-RK; automatic testing and comparison of combustion mechanisms, sensitivity analysis; mechanism optimization). Additional codes are available for assessing the uncertainty of experimental data, mechanism reduction, and global uncertainty analysis.

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P1.22 Binary Co_3O_4–CeO_2 Oxides Supported on Mesoporous Al-Modified SBA-15as Catalysts for Total CH_4 Oxidation

G. Petcu[1], E. M. Anghel[1], S. Petrescu[1], I. Atkinson[1], F. Papa[1], D. C. Culita[1], S. Todorova[2], V. Parvulescu[1]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania
2. Institute of Catalysis, Bulgarian Academy of Sciences, Acad. G. Bonchev St., Bldg 11, 1113 Sofia, Bulgaria

Transition metal oxides are widely recognized as cost-effective and highly active catalysts for the oxidation of air pollutants, including methane and volatile organic compounds. Among them, cerium-based mixed oxides have attracted considerable attention because the incorporation of a second transition metal can generate synergistic effects that enhance redox properties and catalytic performance. In particular, Co_3O_4–CeO_2 mixed oxides have demonstrated excellent activity in oxidation reactions owing to the strong interaction between the two oxide phases. The catalytic performance of these materials is strongly influenced by the nature of the support and the metal–support interactions. In this work, mesoporous SBA-15 was modified with aluminum to tailor its structural and surface properties, aiming to improve the dispersion and reducibility of the active Co_3O_4–CeO_2 phase. Cerium and cobalt were simultaneously introduced onto Al-modified SBA-15 by incipient wetness impregnation using aqueous nitrate solutions, with nominal loadings of 15 wt% Ce and 20 wt% Co. After impregnation, the samples were dried at 80 °C for 8 h, followed by calcination in air at 400 °C for 4 h. Co_3O_4–CeO_2/Al-SBA-15 catalysts with Al contents of 3 and 6 wt% were prepared and subsequently characterized by small-angle X-ray diffraction (XRD), N_2 adsorption–desorption, SEM-EDX, Raman and FTIR spectroscopy, and H_2-TPR. Their catalytic performance was evaluated in total methane oxidation using a continuous-flow fixed-bed quartz tubular microreactor (inner diameter = 6 mm) operated at atmospheric pressure. The feed consisted of an air/CH_4 mixture (10% CH_4, 5% N_2 and 85% Ar) with an air/CH_4 volume ratio of 2:1. The results demonstrate that aluminum incorporation significantly affects the structural and textural properties of the SBA-15 support as well as the reducibility of the Co_3O_4 active phase. These modifications influence the catalytic behavior, leading to different methane oxidation activities depending on the aluminum content. The study highlights

the important role of support modification in optimizing the performance of Co_3O_4–CeO_2/SBA-15 catalysts for total methane oxidation.

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P1.23 Effect of the Silica-Modified Support on the Selectivity of RuO_2/TiO_2 Nanocompositesfor Photocatalytic Reduction of CO_2

G. Petcu[1], F. Papa[1], E. M. Anghel[1], S. Petrescu[1], A. Baran[1], J.-L.Blin[2], V. Parvulescu[1]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania
2. Université de Lorraine, CNRS, L2CM, F-54000 Nancy, France

Nanocomposites are among the most promising materials for future research. TiO_2–SiO_2 composites, in particular, have attracted considerable attention due to the synergistic combination of properties such as mechanical strength, electrical conductivity, optical properties, catalytic and photocatalytic activity, and thermal stability arising from the intrinsic characteristics of their individual constituents [1]. Modification of this semiconductor with noble metals has been widely investigated to enhance its photocatalytic performance. Ruthenium has recently attracted considerable attention because of its unique physicochemical properties. Accordingly, Ru and RuO_2 nanoparticles have been employed in a variety of photocatalytic systems, and their immobilization on TiO_2 has significantly enhanced photocatalytic CO_2 reduction [2]. In this study, a mesostructured silica–titania support was synthesized by the sol–gel method in the presence of the triblock copolymer P123. The mesostructured SiO_2–TiO_2 supports were obtained after surfactant extraction with ethanol, followed by calcination at 350 °C. The supports were subsequently impregnated with different Ru loadings (1, 3 and 5 wt%), dried, and calcined at 350 °C. The resulting photocatalysts were characterized by SEM, CO_2-TPD, H_2-TPR, Raman, UV–Vis, and photoluminescence spectroscopy.The photocatalytic performance of the obtained materials was evaluated for CO_2 reduction using water as the hydrogen source under visible-light irradiation (525 nm). CO_2-TPD analysis showed that modifying TiO_2 with a small amount of silica (2.5%) optimized the surface for more efficient interaction with CO_2 molecules. SiO_2 acts as a dispersing agent, increasing the specific surface area and providing a greater number of active adsorption sites. Furthermore, the presence of SiO_2 may promote the formation and stabilization of oxygen vacancies. The synthesized nanocomposite materials exhibited photocatalytic activity for CO_2 reduction under visible-light irradiation. The highest CO_2 conversion was achieved for the sample containing 5 wt% Ru supported on the calcined support. These results demonstrate the influence of Ru loading and support treatment on CO_2 conversion. Moreover, product selectivity was strongly influenced by the presence of SiO_2, which modified the support properties and favored methanol production over methane formation. In conclusion, the results demonstrate that the selectivity of photocatalytic CO_2 reduction over Ru-supported SiO_2–TiO_2 composites strongly depends on the properties of the metal co-catalyst, surface hydrophobicity, and metal–support interactions.

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P1.24 Supported Iridium Catalysts for Total Methane Oxidation.Effects of Modified Zeolite Y and SBA-15 Supports

G. Petcu, S. Petrescu, E.M. Anghel, I. Atkinson, F. Papa, D. C. Culita, V. Parvulescu
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania

Iridium catalysts have been less extensively investigated than other noble metal catalysts, although they show promising activity in the oxidative degradation of pollutants [1], including volatile organic compounds (VOCs), while being less expensive than Au- or Pt-based catalysts. In the present study, iridium-based catalysts were synthesized to investigate the effect of the support on their catalytic activity. Iridium catalysts (0.5 wt% Ir) were prepared by incipient wetness impregnation of Al-modified SBA-15 [2] and Ti-modified zeolite Y [3] using an $IrCl_3$ solution, followed by drying and calcination in air at 600 °C for 4 h. Four catalysts, denoted IrSB, IrAlSB, IrZY, and IrTiZY, were obtained and characterized by X-ray diffraction (XRD), nitrogen adsorption–desorption, SEM coupled with EDX, Raman spectroscopy, and H_2-TPR. The catalytic performance was evaluated in the total oxidation of methane, used as a

model air pollutant. During the catalytic tests, the bed temperature was increased from 200 to 500 °C. Small-angle X-ray diffraction confirmed the well-ordered mesostructure characteristic of SBA-15. The degree of structural ordering was only slightly affected by aluminum incorporation (3.6 wt%). A similar behavior was observed for zeolite Y, where titanium incorporation (2 wt%) caused only minor changes in the crystalline structure, as evidenced by wide-angle XRD. In both cases, only negligible changes in the adsorption–desorption isotherms and a slight decrease in the specific surface area were observed. SEM images revealed the typical morphologies of SBA-15 and zeolite Y, which were preserved after iridium impregnation. The presence of iridium was confirmed by EDX analysis. Although the Raman spectra exhibited a small shoulder at approximately 530 cm^{-1}, assigned to the Eg vibrational mode of the IrO_2-rutile phase and overlapping with the intense band of the four-membered SiO_4 rings centered at approximately 500 cm^{-1}, no B2g band at around 720 cm^{-1} was observed for the IrAlSB sample. The methane conversion at 500 °C followed the order: IrTiZY>IrZY>IrAlSB>IrSB. In conclusion, the obtained results demonstrate that, similarly to other supported noble metal catalysts, the nature of the support influences the electronic structure of iridium and consequently its catalytic activity toward the total oxidation of methane.

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P1.25 Volumetric, Acoustic and Optical Behaviour for sec-Butylbenzene + Some Binary Liquids Mixtures, in the Range of Normal Temperatures and Pressures

*Florinela Sîrbu, Dana Drăgoescu**
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania.
Corresponding authors: sflorinela@yahoo.com,ddragoescu@icf.ro

The thermophysical properties for two binary mixtures of sec-butylbenzene with some organic liquids, namely sec-butylbenzene + 1-chlorohexane and sec-butylbenzene + iso-propylbenzene, were measured. Experimental data for densities, speeds of sound, refractive indices, and viscosities, at several temperatures in the range of (293.15 to 318.15) K and p = 0.1 MPa, are obtained. By using the obtained results, the deviation and excess properties as: the excess molar volumes, partial/apparent molar volumes, the isentropic compressibilities, the excess molar isentropic compressibilities, as well as the deviation in refractive indices, and the excess molar refractions, have been computed and presented at T = 298.15 K in this work.
All the thermodynamic properties have been correlated with the Redlich-Kister polynomial equation.
The experimental and calculated results are discussed in terms of molecular interactions and structural effects between components of mixtures.

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P1.26 The Versatility of Spectroscopic Ellipsometry. Correlation with Complementary Characterization Techniques

H. Stroescu, M. Gartner, M. Nicolescu
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy,202 SplaiulIndependentei, 060021 Bucharest, Romania

Spectroscopic ellipsometry (SE) is a powerful, non-destructive and non-contact technique for the optical characterization of thin films, working both ex situ and in situ. It is a comprehensive technique that provides valuable information about the chemical, structural and electrical properties of the studied films.
The utility of SE is shown by its ability to substitute alternative characterization techniques such as XRD, TEM, AFM, UV-Visspectroscopy, and Hall Effect measurements. While these methods are often expensive and complex, ellipsometry offers a highly efficient, rapid and cost-effective alternative to these techniques.
On the other hand, a complex ellipsometric analysis can also give information about the film porosity and anisotropy, while providing thickness and optical uniformity mapping, optical constants across the entire film and precise data on bowing parameters.
In this work, several representative examples illustrating the correspondence between SE results and independent characterization methods are presented.
The structural information obtained for $TiO_2(Ni^{2+})$ sol-gel films by X-ray diffraction (XRD) is correlated with features observed in the ellipsometric spectra. The formation of anatase and rutile phases following thermal treatment is reflected in the spectral response measured by SE, with the corresponding phase assignments confirmed by XRD.

The optical characterization of nanocrystalline ITO multilayer films provides another example, with refractive index values obtained from SE in good agreement with those from optical transmission measurements.
Also, the thickness determined by SE for Nb-doped TiO_2 sol-gel films (339.9 nm) shows a good agreement with the value obtained by cross-sectional transmission electron microscopy (XTEM, 340 nm).
In the case of sol-gel nanocrystalline ITO multilayer films obtained by successive sol–gel spinning deposition, the SE data are well fitted using the structural model provided by XTEM, with a good delimitation of the layers and crystallite size of 10–20 nm.
ITO sol–gel thin films deposited on glass, SiO_2/glass, and SiO_2/Si substrates were successfully characterized using Infrared Spectroscopic Ellipsometry (IRSE) and Raman spectroscopy. The vibrational modes of all three film types were identified, demonstrating a good agreement between the two techniques.
The examples presented in this work demonstrate the versatility of spectroscopic ellipsometry. The correlation of SE with structural, optical and electrical characterization techniques provides complementary information and contributes to a more comprehensive understanding of thin-film properties.
A future challenge in ellipsometry is the development of data bases of polymer and organic materials with applications in biology and medicine.

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This study was conducted in the framework of the research program “Surface Chemistry and Catalysis” of the “Ilie Murgulescu”Institute of Physical Chemistry of the Romanian Academy.

P1.27 Thermodynamic Descriptors of the Entropy-Stabilized Oxides: A Case Study on Rocksalt Entropy-Stabilized Oxide (Co,Cu,Mg,Ni,Zn)O

S. Tanasescu[1], F. Teodorescu[1], C. Marinescu[1], A. Sofronia[1], A. Botea-Petcu[1], F. Maxim[1], M. C. Licu[1], C. Hornoiu[1], D. Berardan[2], N. Dragoe[2]*
1. Ilie MurgulescuInstitute of Physical Chemistry of the Romanian Academy
2. ICMMO (UMR 8182 CNRS), Université Paris-Saclay, 91405 Orsay, France

Due to their unique and highly tailorable functional properties, there is an increasing interest in high entropy ceramics and, particularly, in the area of entropy-stabilized oxides. One of the key parameters responsible for the relationship composition-structure-properties is the change of the energetic parameters. In order to find new ways to tune, enhance and optimize the properties of novel entropy-stabilized materials designed for different applications, the thorough knowledge of the thermodynamics of the new materials is essential. The focus of our present research is to give insights into the relevant thermodynamic functions suitable for evaluation of the thermodynamic stability in particular temperature ranges associated with the structural changes during heating of the rocksalt entropy stabilized oxide (Co,Cu,Mg,Ni,Zn)O. The energetic parameters obtained in a large temperature range by several experimental methods, in both isothermal and dynamic regimes (Drop Calorimetry, Solid State Electromotive Force Measurements, TG/DSC), have been analyzed. The partial molar energy, enthalpy, and entropy values of oxygen dissolution in the crystalline phase were evaluated for the first time [1] and the relationship of the thermodynamic stability with changes in anionic defect structure has been revealed. Further, by integrating findings from thermal expansion and electrical conductivity measurements, the strong interplay between the thermodynamic properties and electrical, thermomechanical, and structural characteristics is emphasized, the thermodynamic parameters emerging as key descriptors of the metastable to single phase transformation. This is especially important as the materials deriving from this prototypical entropy-stabilized compound are of great interest for energy storage and conversion applications, the understanding and control of their thermodynamics being essential to find new routes for modifying the properties using various substitutions by several aliovalent elements, and creating vacancies in the oxygen sites.

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P1.28 Development of a New Optimised H_2 Combustion Mechanism Using a Large Experimental Data Collection

Ilya E. Gerasimov[1,2],Tibor Nagy[3], Máté Papp[1], Tamás Turányi[1], Alexander A. Konnov[4]
1. Institute of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary
2.Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia
3. Institute of Materials and Environmental Chemistry, HUN-REN Research Centre for Natural Sciences, Budapest, Hungary

4. Division of Combustion Physics, Lund University, Lund, Sweden

The transition to renewable energy is essential for reducing the environmental impact of fossil fuels. While solar and wind power enable electricity generation with minimal carbon emissions, several sectors – such as heavy transportation, shipping, and energy-intensive industries – remain difficult to electrify. In these areas, alternative fuels such as hydrogen, ammonia, and biomass offer promising solutions. The advancement of combustion technologies requires a detailed and accurate understanding of the combustion chemistry of these fuels. Hydrogen is particularly important because its elementary reactions form the core of the high-temperature combustion mechanisms for a wide range of fuels, including hydrocarbons, oxygenates, and ammonia-based fuels. As a result, hydrogen combustion schemes and their associated reaction rate constants are continuously refined, and new experimental measurements in hydrogen flames are regularly published. With the availability of extensive recent datasets and advances in mechanism optimisation methods, there is a clear opportunity to develop a modern hydrogen combustion mechanism that is predictive across a broad range of conditions.

The updated version of the hydrogen mechanism proposed by Konnov [1] has shown a very good performance in a hydrogen mechanisms evaluation study against an updated collection of 7334 experimental data points, which included measurements of ignition delay times (IDT), laminar burning velocities (LBV), and species concentrations (SPEC) in flames, jet-stirred, and flow reactors for neat hydrogen. Therefore, it was selected as the basis for the development of a new hydrogen combustion mechanism. After evaluating the uncertainties in the rate constants for the most important reactions identified by sensitivity analysis, the PCALIN algorithm [2] identified 29 reactions requiring revision. The corresponding rate parameters (Arrhenius A factors and third-body efficiency parameters) were optimised within their prior uncertainty limits.

Although the updated Konnov mechanism performed very well in LBV and IDT simulations, it showed considerable deficiencies in other types of experiments, particularly in simulations of jet-stirred reactor species concentration measurements. The optimisation of the modified Konnov mechanism was performed using a subset of the full experimental data collection, comprising the most reliable measurements across all available experimental conditions. Subsequently, the optimised mechanism was tested on the full data collection and demonstrated improved performance.

The optimised mechanism outperforms all previously published hydrogen combustion mechanisms across a wide range of experimental conditions and experimental types. The mean-squared error function value E was 12.4 and 9.6 for the initial and the optimised mechanism, respectively. The new model can be used to simulate a wide variety H_2 combustion systems and be integrated into the combustion mechanisms for other fuels.

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Poster Session 2

Day 2 — Wednesday, 24 September · 10:00 – 15:00 (Interactive Discussions, Continuous Exhibition, ROMPHYSCHEM 18th edition)

Molecular Design & Resilience; Heritage Conservation and Environmental Initiatives; Future of Ecosystem Solutions — Frontiers in Molecular Science for Environmental Resilience

P2.01 The Influence of Divalent Cations and Host-Guest Interactions on the Properties of Functionalized Alginate Gels

Elena E. Antonia[1], Gabriela Ionita[1], Carmen M. Topală[2], Alexandru-Gabriel Bucur[1], Mihaela L. Ciutu[1], Elena N. Hristea[1], Rodica D. Baratoiu (Carpen)[1], Ludmila Aricov[1], Anca-Ruxandra Leontieș[1]

1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Faculty of Sciences, Physical Education and Computer Science, The National University of Science and Technology Politehnica Bucharest, Pitesti University Centre, 1 Targu din Vale Street, 110040 Pitesti, Romania

Alginate-based hydrogels constitute a versatile class of polymeric materials whose properties can be tailored through ionic cross-linking and the incorporation of supramolecular interactions. The coordination between divalent cations and alginate chains constitutes a determining factor in the structural organization and mechanical behavior of the resulting hydrogel network. In the present study, the influence of various divalent cations on alginate gelation was investigated, together with the effect of host-guest interactions introduced via adamantyl and β-cyclodextrin functionalization. Electron paramagnetic resonance (EPR) spectroscopy was employed to elucidate the local molecular environment and rotational dynamics of paramagnetic moieties within the polymer network.

Alginate was functionalized with 4-amino-TEMPO, while additional systems containing adamantyl groups and β-cyclodextrin units were investigated in order to assess the contribution of host-guest interactions to network formation. Hydrogels were obtained through ionic cross-linking using Ba^{2+}, Ca^{2+}, Sr^{2+}, and Zn^{2+} ions. The resulting systems were characterized by EPR and infrared (IR) spectroscopy, complemented by rheological measurements. EPR spectra were analyzed in terms of the nitrogen hyperfine splitting constant (a_N) and the effective $2A_{zz}$ parameter, used to evaluate the local mobility and immobilization of the spin-labeled moieties.

The nature of the divalent cation strongly influenced both the rheological and EPR properties of the alginate hydrogels. Rheological measurements revealed predominantly elastic behavior, with Ba^{2+} producing the strongest networks, while Zn^{2+} resulted in softer gels. A similar trend was observed by EPR, with the effective $2A_{zz}$ values decreasing in the order $Ba^{2+} > Ca^{2+} > Sr^{2+} > Zn^{2+}$, indicating progressively less restricted motion of the paramagnetic moieties. The incorporation of β-cyclodextrin and adamantyl groups further modified the local dynamics through host-guest interactions. Notably, the β-cyclodextrin-containing systems exhibited increased $2A_{zz}$ values, consistent with enhanced immobilization of the spin probes. Taken together, the spectroscopic and rheological results demonstrate that EPR spectroscopy provides valuable local-scale information complementary to the macroscopic mechanical characterization of alginate-based hydrogel networks.

P2.02 Multilayered Polymer-PET Hybrid Supports for Enhanced Enzyme Immobilization

Ludmila Aricov[1], Raluca-Marieta Toma[1], Adriana Băran[1], Adina Răducan[2], Anca-Ruxandra Leontieș[1]*

1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Department of Physical Chemistry, Faculty of Chemistry, University of Bucharest

Corresponding author: aricov_ludmila@yahoo.com, laricov@icf.ro

The increasing contamination of water resources with textile dyes has created an urgent need for efficient, sustainable, and environmentally friendly treatment technologies. Enzymatic processes using oxidative enzymes like laccase (Lc) from Trametes versicolor offer high catalytic efficiency and biodegradability under mild conditions, yet their large-scale application is limited by high production costs, structural instability, and recovery challenges. To overcome these limitations, this study presents the development of a polyethylene terephthalate (PET) support coated with chitosan (CS) and polyacrylic acid (PAA) multilayers for the immobilization of Lc. Following PET surface functionalization with carboxyl groups, layer-by-layer assembly of CS/PAA multilayers provided a suitable functional interface for enzyme immobilization via 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC) activation. The resulting biocatalyst exhibited enhanced surface properties and catalytic performance during ABTS oxidation. Surface functionalization significantly increased material hydrophilicity, with the water contact angle decreasing from 89.56° for PET to 57.03° for carboxylated PET, reaching 33.46° for the immobilized product. Increasing the assembly from one to five CS/PAA bilayers led to an approximately 3.2-fold rise in the reaction rate. Furthermore, the immobilized Lc demonstrated enhanced pH stability, retaining high residual activity over the investigated range with maximum efficiency at pH 3, while displaying good reusability by retaining approximately 81% of its initial activity after five consecutive oxidation cycles. The PET-COOH/CS/PAA/Lc system serves as a highly promising support for wastewater remediation, combining improved stability and excellent reusability.

P2.03 Host–Guest Complexation of β-Phosphorylated Nitroxide Radicals with Cyclodextrins: Effects of Stereochemistry, Functionalization and Ionic Strength

Alexandru-Gabriel Bucur[1], Sylvain R. A. Marque[2], Gabriela Ionita[1]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Aix Marseille Université, CNRS, ICR, UMR7273, Marseille 13397, France

Host-guest chemistry of stable radicals has been extensively investigated by electron paramagnetic resonance (EPR) spectroscopy, with most studies focusing on the inclusion of nitroxides in cyclodextrins (CDs). Here, we investigate the complexation of a series of β-phosphorylated cyclic nitroxide radicals with β-cyclodextrin (β-CD) and γ-cyclodextrin (γ-CD), with particular emphasis on the effects of stereochemistry, functionalization, and ionic strength on host-guest interactions.

The studied radicals include two diastereoisomers bearing a hydroxymethyl substituent, together with the corresponding acetate- and adamantane-functionalized derivatives. Differences in the phosphorus and nitrogen hyperfine splitting constants provide distinct EPR signatures for the stereoisomers, enabling their complexation behavior to be followed directly. In the hydroxyl-substituted pair, the cis stereoisomer can form an intramolecular hydrogen bond between the hydroxyl group and the phosphoryl moiety, whereas this interaction is not accessible to the trans stereoisomer. This structural difference leads to distinct inclusion behavior, particularly with γ-CD, for which the trans stereoisomer exhibits stronger association.

Comparison of the different functional groups further demonstrates that subtle structural modifications markedly influence cyclodextrin recognition. In β-CD, the hydroxyl- and acetate-substituted radicals display comparable complexation behavior, whereas the adamantane-functionalized derivatives show a distinct binding pattern, suggesting inclusion from a different side of the molecule. Binding constants obtained from EPR measurements generally reveal stronger association with γ-CD than with β-CD. In addition, increasing potassium chloride concentration enhances complex stability, highlighting the important contribution of solvation and electrostatic effects to the host–guest equilibrium.

Overall, these results demonstrate that molecular stereochemistry, functionalization, and ionic strength collectively govern the inclusion of β-phosphorylated nitroxide radicals in cyclodextrins and provide insight into the rational design of tunable supramolecular spin systems.

P2.04 The Influence of Polyphenol on Hemoglobin Thermal Stability

*Alexandra Busuioc, Vlad Tudor Popa, Aurica Precupas**
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
Corresponding author: aprecupas@icf.ro

The study of polyphenol influence on protein thermal stability is a promising approach concerning amyloid formation, with a wide range of applications in the medical and biotechnology fields. The effect of different concentrations of quercetin (QUER), a plant flavonoid with antioxidant, anti-inflammatory, antibacterial, antiviral activity on bovine hemoglobin (BHb) conformation and thermal stability was investigated using differential scanning microcalorimetry (μDSC), circular dichroism (CD), dynamic light scattering (DLS), Thioflavin T (ThT), Congo Red, and 8-Anilino-1-napthalenesulfonic acid (ANS) binding assays. Quercetin acts as a concentration- and incubation temperature-dependent modulator of protein aggregation. μDSC measurements reveal that low concentrations of polyphenol slightly stabilize the BHb structure, whereas higher concentrations promote aggregation. Following prolonged incubation at physiological temperature, QUER acts as a promoter of BHb aggregation, as evidenced by calorimetric and spectroscopic methods. CD results point to the increase in β-sheet content observed in the presence of polyphenol, indicating formation of protein aggregates. The presence of oligomeric species and larger aggregates detected by DLS, together with the results of Congo Red, ThT, and ANS assays, suggest that QUER influences both protein unfolding and the subsequent aggregation. The polyphenol binds within the central cavity of native BHb through hydrogen bonds and hydrophobic interactions. This study provides insightful information concerning the influence of polyphenol on protein thermal stability with potential applications in biomaterials science and biopharmaceutical formulations.

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P2.05 Unexpected Rearrangement of Phenoxypicramide to 1,3-Dinitro-10H-phenoxazine

Rodica D. Carpen (Baratoiu)[1], Elena N. Hristea[1], Petre Ionita[2]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. University of Bucharest, Faculty of Chemistry, 90 Panduri, Bucharest 050663, Romania

The attempt to obtain phenoxypicramide from a classical nucleophilic substitution reaction using as reagents phenoxyamine and picryl chloride unexpectedly led to the formation of 1,3-dinitro-10H-phenoxazine. The mechanism of formation, involving a molecular rearrangement with expelling of a nitro group, is discussed. ^{1}H-NMR, ^{13}C-NMR, IR, ESI-MS, and UV-Vis spectra; X-ray molecular structure for synthesized compound are also presented.

P2.06 Synthesis of Nitronyl Nitroxide with Alkylchains and Analysis of Their Behaviour in SDS Micelles in the Absence and Presence of GSH

Rodica D. Carpen (Baratoiu), Elena N. Hristea, Alexandru V. F. Neculae, Alexandru G. Bucur, Mihaela L. Ciutu, Sevasti Matsia, Gabriela Ionita
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

In this study, a series of nitronyl nitroxide (NN) radicals functionalized with alkyl chain (C3, C4, C6, C8, C9 and C10) was obtained. Radical behavior was monitored in aqueous media and sodium dodecyl sulfate (SDS) micelles. Accessibility properties and micellar partitioning of all radicals were evaluated in a concentration-dependent manner, using Electron Paramagnetic Resonance (EPR). Glutathione (GSH) reactivity and quantitative EPR kinetic analysis revealed that the reduction rate constants systematically decrease with increasing alkyl chain length, leading to the formation of diamagnetic hydroxylamine species. In the presence of SDS, the reactivity of NN derivatives with GSH was dramatically suppressed, confirming the protection of nitroxide center from thiol reduction.

P2.07 Attributes of C and N Natural Abundances and the Stoichiometry of Extractable Nutrients as Influenced by Different Land Use Types: Application of Stable Isotopes

*Achalu Chimdi[1], Geshere Abdisa Gurmesa[2], Ang Wang[2], Yunting Fang[2]**
1. School of Natural Resources, Ambo University, Ambo, Ethiopia
2. Institute of Applied Ecology, Chinese Academy of Sciences, Shenyang, China
Corresponding author: fangyt@iae.ac.cn

Understanding the transformation of soil nutrients and characteristics of ecological stoichiometry in soils is vigorous in sustainable land management and ecosystem health. This study characterized the soil carbon(C), nitrogen (N) natural abundances and stoichiometric relationships of C, N, P (phosphorus), extractable nutrients of potassium (K), zinc (Zn), manganese (Mn), nickel (Ni), copper (Cu), and chromium (Cr) across various land uses and soil depths of Jeldu District, West Showa zone, Oromia, Ethiopia. The samples collected from different land use types and soil depths in 2025 were analyzed for soil pH, cation exchange capacity (CEC), available P, total P, extractable nutrients, C, N concentrations, natural abundances of δ^{13}C, and δ^{15}N isotopes using their corresponding standard laboratory procedures and instruments. It had been shown that there are decreasing trends in soil pH, CEC, TP, and extractable K were revealed from soils of (forest → grazing → cultivated) lands. The concentrations of C, N in the litter layer have shown significant variations with increasing soil depths. Similarly, the total N, C, and N concentrations, ratios of C: N and N: P has also shown significant variation across different soil depths of forest land and at 0-20 cm depth of other land uses, whereas the values of δ^{13}C and δ^{15}N isotopes didn`t show significant variation. These findings indicate that the litter layer of forest land holds higher levels of soil C, N concentrations, total N, C: N, and N:P, and some extractable nutrients than other land uses and deeper soils. Our study details that variations in land use types and soil depths were found to be the main indicators that control the contents, stoichiometric features, dynamics, and natural abundances of soil nutrients. Furthermore, this study enhances an understanding of soil C and N natural abundance and stoichiometric ratios across land uses and soil depths and provides comprehensions for sustainable management of soil nutrients, natural resources and health of the ecosystem.

P2.08 Halogenated Nitronyl-Nitroxide Derivatives in Host–Guest Systems

Mihaela L. Ciutu, Gabriela Ionita, Alexandru-Gabriel Bucur, Georgiana A. Sanda, Alexandru V. F. Neculae, Florența D. Savonea
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

Nitronyl nitroxide (NN) radicals are characterized by an unpaired electron delocalized over an N–O···N–O fragment, which confers them high stability and distinct EPR properties. Because their EPR signal is highly sensitive to the local environment, NN radicals are widely used as spin probes to investigate host–guest interactions with macrocyclic hosts. In this work, a series of aromatic NN radicals bearing fluorine, chlorine, and bromine substituents were used to

compare the inclusion behaviour of two structurally different macrocyclic hosts: cyclodextrins (β-CD, γ-CD and HP-γ-CD) and cucurbit[7]uril (CB[7]).
The halogenated NN derivatives were obtained by reaction of 2,3-bis(hydroxylamino)-2,3-dimethylbutane with the corresponding halogenated benzaldehydes (2-chloro-, 2,3-dichloro-, 4-chloro-, 3-bromo-, 4-bromo-, and 2-fluorobenzaldehyde) characterized by EPR. All derivatives display the characteristic five-line EPR spectrum (intensity ratio 1:2:3:2:1) arising from the two equivalent nitrogen nuclei. Their capacity to form inclusion complexes was evaluated in aqueous solutions of increasing host concentration cyclodextrins (β-CD, γ-CD and HP-γ-CD) in one study and CB[7] in the other by monitoring the changes in the hyperfine splitting constant (a_N) and the rotational correlation time (τ) obtained from spectral simulation.
With cyclodextrins, the a_N and τ values of the aromatic NN derivatives change progressively as the host concentration increases, indicating the formation of inclusion complexes; the extent of the change depends on the size and substitution of the cyclodextrin cavity (β-CD, γ-CD and HP-γ-CD), with the chlorinated and brominated derivatives generally showing the most pronounced spectral evolution. With CB[7], by contrast, the EPR response depends strongly on the identity of the halogen atom itself: the fluorinated and chlorinated derivatives show only small spectral changes upon CB[7] addition, whereas the brominated derivative displays pronounced modifications and a distinct signal assigned to the inclusion complex.
Taken together, these results show that the two macrocyclic hosts probe halogen substitution in different ways: cyclodextrin complexation is governed mainly by cavity size and geometric complementarity, while CB[7] complexation is governed mainly by the polarizability and size of the halogen substituent, becoming clearly detectable only for the bromine-substituted guest. This comparison highlights how host architecture determines which structural features of a spin probe are best resolved by EPR spectroscopy.

P2.09 Titanium and Titanium Alloys OrthopaedicImplants

Mihai Marian Radu, Silviu Iulian Drob, Cora Vasilescu*
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
Corresponding author: sidrob@icf.ro

This research study presents the benefits and improvements of the bare Titanium and its alloys designed for orthopaedic implants. The development of Titanium alloys for long term orthopaedic implants should take into account only non-toxic and non-allergenic elements with very high corrosion resistance in bio-electrolytes that do not release any ions or compounds into surrounding tissues and they have a low density and elastic modulus with GPa values close to those of the human bone. Best biocompatible alloying elements are Niobium, Zirconium, Tantalum, Molybdenum, and Tin.
The Titanium alloys were cast using the cold crucible levitation melting (CCLM) under protective argon atmosphere. The ingots obtained were cold rolled until a reduction in thickness of about 95% was achieved.
The bare Titanium and the Titanium alloys were evaluated for their in vitro and corrosion properties. The cytocompatibility was determined according to the ISO 10993-5 assay, which uses the direct-contact method. Their surface was analyzed by SEM, XPS and XRD.
Using a Radiometer Analytical VoltaLab PGZ 402 potentiostat, Titanium and the Titanium alloys were subjected to the following corrosion tests: open circuit potential, electrochemical impedance spectroscopy (EIS), and polarisation for corrosion (Tafel). The results were delivered with the aid of the VoltaMaster 4 program.
The materials and characterisation techniques, assay of cell vitality and corrosion tests indicate that the Titanium alloys designed for orthopaedic implants exhibit very promising properties for their intended role.

P2.10 Comparative Spectroscopic Investigation of Mitoxantrone and Quinizarin Interactions with SDS Micellar Aggregates

Mirela Enache, Ana Maria Toader, Izabella Dascalu
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

The interaction of anthraquinone-based drugs with membrane-mimetic systems is essential for understanding their transport, localization, and pharmacological behaviour. In this comparative spectroscopic investigation, the interactions of mitoxantrone and quinizarin with sodium dodecyl sulfate (SDS) micellar aggregates were analysed by UV–Vis absorption spectroscopy over the temperature range 293.15–323.15 K combined with conductometric measurements.
Both compounds exhibited significant spectral changes upon the addition of SDS, confirming their incorporation into micellar aggregates. Quantitative analysis was performed through the determination of binding constants (Kb), micelle/water partition coefficients (Kx), and the corresponding thermodynamic parameters [1, 2]. Quinizarin displayed stronger binding and higher partition into SDS micelles than mitoxantrone, despite the latter possessing positively charged amino side chains at physiological pH. The difference is attributed primarily to the smaller molecular size and more favourable accommodation of quinizarin within the micellar interface.

Thermodynamic analysis revealed distinct interaction mechanisms: quinizarin binding and partition were spontaneous, endothermic, and entropy-driven, indicating the predominance of hydrophobic interactions, whereas mitoxantrone interactions depended on its ionization state. At pH 7.4, mitoxantrone exhibited an initial electrostatic interaction with SDS monomers followed by incorporation into micelles, with binding governed mainly by enthalpic contributions, while at pH 10 the interaction became predominantly entropy-controlled.
These comparative results provide new insights into the role of molecular structure, charge, and hydrophobicity in drug–micelle interactions and contribute to a better understanding of anthraquinone-based anticancer drug behavior in membrane-mimetic environments, with potential implications for drug delivery system design.

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P2.11 Shaken, Not Stirred: When the Solvent Mediates the Relationship between Pseudopolymorphs of a New Chiral Copper(II) Complex

Cristian D. Ene[1], Catalin Maxim[2,3]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Faculty of Chemistry, University of Bucharest, 4-12 Regina Elisabeta Blvd, 030018 Bucharest, Romania
3. "Costin D. Nenitescu" Institute of Organic and Supramolecular Chemistry of the Romanian Academy, 202B SplaiulIndependentei, 060023 Bucharest, Romania

The way a mononuclear complex entity packs itself in a crystal strongly influences the characteristics of the bulk material, starting from its behaviour at subsequent dissolution and ending up with the interaction nature and the parameter values defining the optical and magnetic properties. Hence, the key to tuning these features relies not only on mastering the triggers that determine the toggling from one arrangement to another, but also on mapping the specific conditions under which such a process occurs. For example, it is not necessary for a given solvent to act as a guest molecules or even a ligand to favour the formation of a certain polymorph, on the contrary, it can only keep it simple by being just the solvent. Here we try to elucidate the protean case of a coordinative compound based on copper(II) and a R- or S-methionine-containing tridentate ligand for which we have identified four of its crystallographic packings so far.

P2.12 Spectroscopic Characterization of C3-Symmetric Pyrene-Based Charge Transfer Complexes Capable of Forming Tunable Organogels

Adrian Gainar[1], Thanh-Loan Lai[2], Cristina Oliveras-Gonzàlez[2], Flavia Pop[2], Matthieu Raynal[3], Benjamin Isare[3], Laurent Bouteiller[3], Mathieu Linares[4,5], David Canevet[2], Narcis Avarvari[2], Marc Sallé[2]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. MOLTECH-Anjou Laboratory, University of Angers, Angers, France
3. CNRS, Institut Parisien de Chimie Moléculaire, Polymer Chemistry Laboratory, Sorbonne University Paris, France
4. Laboratory of Organic Electronics and Group of Scientific Visualisation, ITN Linköping University, Norrköping, Sweden
5. Swedish e-Science Research Center (SeRC), Linköping University, Linköping, Sweden

Supramolecular gels constitute a class of soft materials composed of low-molecular-weight gelators with the capability to assemble in three-dimensional fibre networks in which solvent molecules can be confined. Their applications are present in various domains such as organic electronics, photoconductivity, sensing and pharmacy. Electron donor (D) – electron acceptor (A) two-component organogels and xerogels derived from a C3-symmetric pyrene-containing low-molecular-weight gelator were systematically investigated through a comprehensive multi-technique characterization approach comprising variable-temperature (VT) ^{1}H-NMR, infrared, VT UV-visible and fluorescence spectroscopies, scanning electron and polarizing optical microscopies, TGA, DSC and nanoDSC. The gelation behavior observed by naked eye through color changes was found to be governed by the formation of charge-transfer (CT) complexes between the pyrene moiety D and a series of dopants A. The nature of the dopant molecule proved to be an important parameter with a pronounced influence on the gelation domains, critical gelation concentrations, gel-to-sol transition temperatures, and the microstructures of the resulting xerogels. A remarkable correlation was established between the phase transition temperatures and the thermal disappearance of the characteristic CT absorption bands, directly linking supramolecular organization to the strength of electronic interactions. These findings demonstrate the spectroscopic tunability of these stimulus-responsive supramolecular materials through the nature of donor-acceptor interactions.

P2.13 Advanced Biomaterials Based on Hydrogels Enriched with Natural Essential Oil as Wound Dressings

Adrian Gainar[1], Daniela Cristina Culita[1], Irina Atkinson[1], Jeanina Pandele-Cusu[1], Emma Adriana Ozon[2], Adina Magdalena Musuc[1]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Faculty of Pharmacy, 'Carol Davila' University of Medicine and Pharmacy, 6 Traian Vuia St., 020956 Bucharest, Romania

Hydrogel-based materials derived from renewable biological sources are gaining a growing interest in the recent years as sustainable alternatives to synthetic biomaterials, due to their superior biocompatibility, enhanced antibacterial properties and wound healing capabilities. Within this class, biopolysaccharide-based hydrogels are recognized for their proven biodegradability and biocompatibility, making them attractive for various applications such as tissue engineering, drug delivery, and wound dressings [1]. They can ensure a moist environment favorable to cell migration and proliferation, compared with antibiotics. Carrageenan, extracted from marine red algae, is a naturally sulphated, hydrophilic linear polysaccharide whose properties depend on the number and position of sulfate groups on its repeating unit. Among the different types of varieties, κ-carrageenan is particularly valuable for its strong gelling behavior and film-forming ability, positioning it as a renewable, biobased alternative to synthetic polymers [2]. To enhance the functional performance of the material, lavender essential oil was incorporated for its recognized antimicrobial and bacteriostatic properties [3]. In this work, a κ-carrageenan film loaded with lavender essential oil was developed via physical mixing and homogenization processes as an eco-friendly approach to wound-dressing design. The physicochemical characterization of the dried films showed the structural interaction between κ-carrageenan and essential oil loaded into the polymer network. These findings support the potential of this hydrogel as a biomedical wound dressing, contributing to the development of environmentally friendly healthcare materials.

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P2.14 Pro-Fluorescent Stable Radicals Derived from Amino-Acids

Petre Ionita
University of Bucharest, Faculty of Chemistry, Panduri 90, Bucharest 050026, Romania

Pro-fluorescent stable radicals derived from the amino-acids glycine, beta-alanine, 6-aminohexanoic acid, and 12-aminododecanoic acid were synthesised and characterized. As fluorophore was used the NBD moiety, while as the stable free radical the TEMPO part was employed. Besides, by reacting NBD-chloride with 4-amino-TEMPO, the corresponding pro-fluorescent derivative was obtained and compared with the newly synthesis one. All these derivatives are intense coloured compounds, showing an absorbance band around 465 nm, and a fluorescence band around 540 nm. The intensity of the fluorescence increased several folds by adding a reducing agent, like ascorbic acid. This reduces the nitroxide moiety to the corresponding hydroxylamine, thus restoring the full fluorescence potential. Depending on their structure, characterization was performed by UV-Vis and fluorescence, ^{1}H- and ^{13}C-NMR, ESI-MS, and ESR. Such pro-fluorescent stable free radicals can find applications in many domains, like chemistry, biology, or materials science.

P2.15 Magnetite-Modified Mesoporous Silica for Drug Delivery Applications

Simona Ioniță, Daniel Lincu, Irina Atkinson, Daniela Culiță, Raul-Augustin Mitran
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

Mesoporous silica materials have attracted considerable interest as drug delivery platforms due to their high specific surface area, tunable pore architecture, chemical stability, and the possibility of tailoring their surface properties [1]. Among them, mesocellular foam (MCF) silica is particularly attractive because of its three-dimensional interconnected pore network and large pore volume, which can facilitate the incorporation and transport of various drug molecules [2]. In this study, a magnetic mesoporous silica system based on MCF silica and magnetite (Fe_3O_4) nanoparticles was investigated as a potential platform for drug delivery. Previous studies have demonstrated the feasibility of incorporating magnetic iron oxide nanoparticles into MCF-type structures while retaining their characteristic porous architecture [3, 4].
Magnetite-mesoporous silica composite was obtained using an in situ procedure, by generating magnetite during the sol-gel synthesis of the mesoporous silica particles. The obtained composite was characterized in terms of its textural, thermal, and structural properties. Nitrogen adsorption–desorption measurements were employed to evaluate the

specific surface area, pore volume, and pore size distribution of the MCF matrix. Thermogravimetric analysis (TGA) was performed to assess the thermal stability of the composite. Powder X-ray diffraction (XRD) was used to investigate the structural characteristics and identify the crystalline iron oxide phase within the amorphous silica matrix. The release profile of a model drug molecule was also investigated to assess the composite feasibility as a drug delivery vehicle.

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P2.16 Spectroscopic Evidence of the Physical Interactions between Copper Acetate and a Carboxyl-Substituted Porphyrin in Solution

Anca Lascu, Ionela Frîngu, Nicoleta Pleşu, Adriana Popa*
Institute of Chemistry "Coriolan Drăgulescu", M. Viteazul Ave. 24, 300223 Timișoara, România
Corresponding author: ancalascu@yahoo.com

Literature extensively documents the use of porphyrins as sensitive optical chemosensors for metal ion detection [1-3]. Beyond sensing, copper acetate complexes—such as those formed with prezatide—play vital biological roles by stimulating collagen synthesis and angiogenesis.
In aqueous environments, copper acetate typically dissociates into copper(II) and acetate ions, with the free cations readily undergoing standard precipitation, redox, or coordination pathways. However, when employing 5,10,15,20-tetra-(4-carboxy-phenyl)-porphyrin (4-COOHPP) as the sensitive probe, the spectroscopic detection of copper acetate deviates from these traditional coordination and quantification models.
Upon dissolution, copper acetate dissociates into aqueous Cu^{2+} cations and CH_3COO- anions. The four central nitrogen atoms of the porphyrin core establish an approximately square-planar environment, donating electron density to accommodate the coordination of copper as an axial ligand. Meanwhile, the physical interactions governing the copper ions and the peripheral carboxyl substituents exhibit a dual nature, combining ionic and coordinative bonding components. Concurrently, electrostatic forces and proton-transfer pathways occur between the dissociated acetate anions and the peripheral carboxylic acid groups of the porphyrin macrocycle.

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P2.17 Electrochemical Sensing of Antioxidants Using a Hybrid Nanostructured Composite Based on Conducting Polymer and Metal Nanoparticles

Mariana Marin[1], Sorina-Alexandra Leau[1,3], Cristian Matei[2], Cecilia Lete[1], Stelian Lupu[3]**
1. Department of Electrochemistry and Corrosion, "Ilie Murgulescu"Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, Bucharest, Romania
2. Department of Inorganic Chemistry, Physical Chemistry and Electrochemistry, National University of Science and Technology Politehnica of Bucharest, 1-7 Polizu Gheorghe, Bucharest, Romania
3. Department of Analytical Chemistry and Environmental Engineering, National University of Science and Technology Politehnica of Bucharest, 1-7 Polizu Gheorghe, Bucharest, Romania
Corresponding authors: stelian.lupu@upb.ro, cecilia_lete@yahoo.com

The detection of biologically relevant antioxidants using electrochemical platforms has attracted growing interest because of their important role in oxidative stress and human health. A hybrid nanostructured material based on PEDOT and Ag nanoparticles (AgNPs) was developed and investigated for the electrochemical sensing of quercetin (QR). The combination of the PEDOT matrix with the electrocatalytic activity and high surface area of Ag nanoparticles resulted in a synergistic effect, enhancing the electrochemical response of the modified glassy carbon electrode. We investigated the electrochemical behavior of QR using cyclic voltammetry (CV) and electrochemical impedance

spectroscopy (EIS). The effect of the hybrid material architecture on the electrooxidation behavior of QR was investigated by comparing the electrochemical responses obtained at the hybrid material-modified and unmodified electrodes. The novel preparation strategy was based on the application of alternating currents with controlled amplitude and frequency. A frequency of 100 mHz was employed for polymer deposition while 50 mHz was used for the in-situ electrodeposition of Ag nanoparticles. The PEDOT-AgNPs-based sensing platform exhibited good analytical performance for the determination of QR, with low LOD and LOQ values of 2.8 µM and 9.5 µM, respectively. The practical applicability of the proposed sensing platform was further demonstrated by QR recoveries ranging from 96.46% to 107.27% in red grape must samples. These values support the good accuracy and reliability of the developed electrochemical platform.
These results demonstrate the potential of the hybrid nanostructured platform based on PEDOT and AgNPs for the sensitive electrochemical detection of QR and highlight the role of the individual components in enhancing the electrochemical response.

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P2.18 Assessing Exciton Coupling in Amyloid-Specific Dyes Bound to Biomacromolecules: the Case of Thioflavin T

Iulia Matei
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

The combined induced circular dichroism (ICD) and time-dependent density functional theory (TDDFT) approach has been successfully applied to determine the conformation of flavonoids bound to native proteins [1]. Here, we demonstrate that the ICD/TDDFT method can be extended to amyloid-specific dyes, using thioflavin T (ThT) as model compound. ThT binding to insulin fibrils and heparin generates distinct optical activity, characterized by monosignate and bisignate ICD bands [2]. These signals originate either from chiral, conformationally restricted ThT monomers or from intermolecular exciton coupling between two ThT monomers bound in close proximity. We perform B3LYP/6-311++G(d,p) calculations to identify the molecular species (monomer or dimer) responsible for the ICD features. The spectral signature of the monomer is analysed with respect to the torsion angle between its molecular fragments. Dimer structures are generated considering different spatial arrangements of monomers in order to systematically document how the relative monomer orientation, interchromophoric distance and degree of intramolecular rotation alter the ICD features. Comparison of the simulated and experimental spectra reveals two different binding mechanisms: insulin fibrils interact with monomeric ThT, whereas heparin accommodates two structurally distinct types of ThT dimers. These results recommend ICD/TDDFT as a reliable method for elucidating the chiroptical properties of amyloid dyes that function as molecular rotors.

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P2.19 Molecular Design of Alkyl Chain Functionalized Nitroxide Spin Probes and Study of Biomolecular Interaction

Sevasti Matsia[1], Iulia Matei[1], Alexandru-Gabriel Bucur[1], Aurica Precupas[1], Jean-Patrick Joly[1,2], Sylvain. R. A. Marque[1,2], Gabriela Ionita[1]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Aix Marseille Université, CNRS, ICR, UMR7273, Marseille 13397, France

Serum albumins are important transport proteins that interact with a wide range of endogenous and exogenous molecules [1], making them valuable models for investigating interactions in a molecular level [2]. In this study, bovine serum albumin (BSA) was employed as a model protein to investigate the molecular interactions and structural effects of six newly designed spin probes. The probes incorporate different nitroxide moieties, including TEMPO, PROXYL and a phosphorylated nitroxide, combined with long alkyl chains positioned either at the terminal or central part of the molecular structure. This systematic molecular design enables the influence of probe architecture, hydrophobicity and functionalization on protein binding and dynamics to be evaluated. Particular attention was given to binding affinity and site preference, probe mobility and insertion depth, as well as possible changes in protein stability and conformation. A complementary experimental and computational approach was applied. Electron paramagnetic resonance (EPR) spectroscopy, supported by non-linear spectral fitting (NLSL), was used to characterize probe mobility and binding behavior. Micro-differential scanning calorimetry (µDSC) evaluated changes in BSA thermal stability, while circular dichroism (CD) spectroscopy monitored alterations in secondary structure. Molecular docking calculations further provided insight into the probable binding sites and molecular interaction modes. By correlating molecular structure with biomolecular binding, dynamics and stability, this work demonstrates how rational molecular design

can be used to understand interactions between functional organic molecules and biological macromolecules. The findings contribute to the broader development of molecular engineered systems for sustainable monitoring applications.

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P2.20 Colloidal Complexes for Cover Alginate Hydrogel Beads Involved in Dyes Adsorption

Raluca-Marieta Toma[1], Monica Elisabeta Maxim[1], Gabriela Stîngă[1], Alina Iovescu[1], Daniel Angelescu[1], Simona Petrescu[1], Ludmila Aricov[1], Anca-Ruxandra Leontieș[1], Cătălina Gîfu[2], Adriana Băran[1], Lavinia Vlaia[3], Ioana Viorica Olariu[3]*
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. National Research and Development Institute for Chemistry and Petrochemistry, ICECHIM, Spl. Independenței 202, Sector 6, 060021 Bucharest, Romania
3. Department II - Pharmaceutical Technology, Formulation and Technology of Drugs Research Center, Faculty of Pharmacy, 'Victor Babeș' University of Medicine and Pharmacy, Timișoara 300041, Romania

This study approaches the interaction between two polysaccharides, namely chitosan (CT) and dextran T10 (Dex), as well as the coating of a calcium alginate hydrogels with the formed colloidal complex and anionic surfactant (SDS). CT and Dex chains are attracted together by H-bonds and some hydrophobic bonds and formed positively charged complexes, which were subsequently confirmed by Surface tension, DLS and Zeta potential. The sequential coated hydrogel beds are characterized by FTIR, and SEM. The UV-Vis spectroscopy was used to analyze the adsorption performance takes into consideration the pH of the solution, dye concentration, $CaCl_2$ concentration (1%, 5% and 10% w/v) and hydrogel mass. The adsorption isotherms fitted with Sips and Freundlich equations confirm that the adsorption of methylene blue (MB) is favorable onto a hybrid homogenous/heterogenous surface with a high adsorption efficiency. The results indicate a new eco-friendly and good natural material for waste water treatment.

P2.21 Conductive and Chiral Metal–Organic Frameworks Based on Redox-Active TTF Ligands

Teodora Mocanu[1,2], Pascale Auban-Senzier[3], I. Olejniczak[4], B. Barszcz[4], Narcis Avarvari[1], Nicolas Zigon[1]**
1. Moltech Anjou UMR 6200 CNRS - Université d'Angers UFR Sciences, 49045 ANGERS, France
2. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependenței, 060021, Bucharest, Romania
3. Université Paris-Saclay, CNRS, UMR 8502, Laboratoire de Physique des Solides, Orsay, 91405, France
4. Institute of Molecular Physics Polish Academy of Sciences Smoluchowskiego 17, 60-179 Poznań, Poland
Corresponding authors: nicolas.zigon@univ-angers.fr, Narcis.Avarvari@univ-angers.fr

Conductive metal-organic frameworks have emerged as promising advanced functional platforms for applications in electrocatalysis, chemical sensing, energy storage, by combining MOFs' well-defined architectures and structural features with electrical conductivity and redox activity [1]. The incorporation of chirality into conductive porous coordination networks provides a versatile platform for next-generation spintronic devices and spin-selective materials [2]. Tetrathiafulvalene (TTF) unit is one of the most prolific electroactive moieties in organic electronics and molecular conductors, owing to its reversible redox chemistry and its ability to promote efficient charge transport through close intermolecular contacts and increased sulfur orbital overlap [3]. Sulfur-rich tetrathiafulvalene–tetrathiapentalene (TTF–TTP) derivatives further enhance intermolecular coupling and charge delocalization, offering a rational strategy to approach metallic transport in crystalline organic assemblies [4] and potentially in coordination networks. The M2TTFTB series (M = Zn, Cd, Co, and Mn) represents a prototypical class of through-space conductive MOFs, in which the metal nodes modulate charge transport by controlling π–π and S···S interactions within helical TTF stacks [5].
Herein, we explore two complementary strategies for developing conductive and chiral TTF-based coordination frameworks. We report the induction of chirality in the M2TTFTB series MOFs (M = Zn, Cd, Mn) by controlled incorporation of enantiopure chiral additives. Post-synthetic metal exchange was further investigated to access the Co(II) and Ni(II) analogues. Additionally, we introduce a novel tetracarboxylic bis-fused TTF ligand, TTF-TTP$(COOH)_4$. Its assembly with alkali metal ions afforded 3D networks, exhibiting electrical conductivities up to 300 S/cm.

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P2.22 Assessment of Antimicrobial Powders Incorporation in Acrylic Resins for Temporary Dentures: Physicochemical Evaluation in the Presence of Lysozyme and α-Amylase

Andreea Neacsu[1], Misu-Marian Babat[2], Ioana Leontina Gheorghe[1]*
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. University of Medicine and Pharmacy "Titu Maiorescu", Faculty of Dentistry, Traian Vuia Str., no. 6, sect. 2, Bucharest, Romania
Corresponding author: addneacsu@icf.ro

Introduction: Dental prostheses for temporary dentures are constantly exposed to saliva, food residues, microorganisms, and mechanical wear. Therefore, they can become favorable surfaces for bacterial and fungal biofilm formation. Temporary prostheses could become an intermediate solution contributing to tissues remodel and heal. If antibacterial powders such as Zinc oxide (ZnO) and Calcium hydroxide ($Ca(OH)_2$) are incorporated into a temporary prosthetic resin, their gradual release in the presence of saliva can be especially beneficial. Saliva acts as a natural aqueous medium that can help dissolve, diffuse, and transport antimicrobial agents from the material surface. ZnO and $Ca(OH)_2$ show strong antimicrobial, antifungal, antiviral, and antibiofilm activity. $Ca(OH)_2$ has been used in dentistry for more than 100 years, especially in endodontics, pulp therapy, and restorative procedures while ZnO was used especially as a filler or modifier in dental composites and cements. Saliva is not just water; it contains proteins, ions, enzymes, and microorganisms. α-amylase, one of the main salivary enzymes, and may influence the interaction between the prosthetic material and the oral environment.
The aim of this study is to evaluate the physicochemical changes occurring as a result of the interaction between α-amylase and different antibacterial prosthetic formulations.
Materials and Methods: For the synthesis of the prosthetic mixture, a provided commercial product was used. This is a powder and liquid system product for the production of dental temporary crowns and bridges and the formulations were done by mixing ratio of 2 weight part powder with 1 weight part liquid. The provided composition of powder is a bead polymer made of polymethyl methacrylate (PMMA), pigments and initiators while the liquid consist in methyl methacrylate, tetramethylene dimethacrylate and diurethanedimethacrylate, initiators and stabilizers. The type of polymerization is a self-curing resin based on dibenzoyl peroxide. $Ca(OH)_2$ and ZnO were used to prepare the mixtures with the prosthetic polymer. Further, equal quantities of dried mixtures of prosthetic polymer (AC) with $Ca(OH)_2$ or ZnO, (AC-$Ca(OH)_2$ or AC-ZnO) were immersed in vials containing equal volumes of alpha-amylase (α-amylase) in saline solution. The obtained results consist in UV-Vis spectroscopic evaluation and in docking results analysis. UV-Vis measurements were done to observe the modification of α-amylase in presence of $Ca(OH)_2$ and ZnO considering the time exposure at AC-Ca(OH)2 and AC-ZnO for 1h, 4h, 8h and 24h. The docking analysis reveal the docking energy score, distance, type of interaction and amino acids involved in the binding site of α-amylase with $Ca(OH)_2$ and ZnO.
Conclusions: Therefore, testing in the presence of α-amylase helps determine whether the modified acrylic resin will remain effective and stable in saline solution. The expelled quantities of $Ca(OH)_2$ and ZnO were monitored. The interaction with amylase shows the extent to which the release of antimicrobial powders can modify natural proteins in saliva and allows the establishment of optimal quantitative formulations to maintain the antimicrobial effect.
The perspectives of this work allow future investigations as the evaluation of the interaction with specific bacterial strains or pathogens and the evaluation of the mechanical properties of the mixture formulations.

P2.23 Beta-Lactoglobulin Thermal Denaturation Kinetics in the Presence of Naringin Using Microcalorimetry

*Daniela Gheorghe, Aurica Precupas, Vlad Tudor Popa**
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
Corresponding author: vtpopa@icf.ro

The thermal behavior of β-lactoglobulin (BLG) – naringin (NRG) mixtures in 20 mM glycine-HCl buffer pH 2.0, at molar ratio NRG:BLG = 0, 1, 10 was investigated by differential scanning calorimetry (TA NanoDSC) means. Seven heating rates within the 0.4–1.6 K/min range were utilized. The obtained data did not reveal the expected monotonous variation of denaturation peak temperatures with heating rate, therefore excluding the application of nonisothermal kinetic methods.
On one hand, this is due to the unfavorable signal-to-noise ratio and to errors in signal integration with sigmoid baseline. On the other hand, the irregular variation of peak temperatures may be caused by the intrinsic (multi stage) complexity of the denaturation process.
An adapted kinetic analysis method advanced by Sanchez-Ruiz et al. [1] evidenced two such stages, depending on conversion (α): one with higher activation energy at low α, the other with lower activation energy at high α. However,

in spite of the excellent quality of the corresponding fits, one may expect a certain degree of arbitrariness in the choice of the temperature range of the two stages.
Consequently, an alternative procedure was adopted: all experimental runs were analyzed within the conversion range $0.05 < \alpha < 0.95$, with some loss in fit quality compensated by the gain in objectivity. The averaged (over heating rates) values of apparent activation energies obey the rule:

$$E_{NRG:BLG=0} \leq E_{NRG:BLG=10} < E_{NRG:BLG=1}$$

The above relationship represents a kinetic expression of frequently reported ”counteraction” of the excess ligand on protein thermal behavior: while bound ligand (1:1 molar ratio) stabilizes the protein, excess (free) ligand exerts an opposite action.

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P2.24 Zein–Resveratrol Interactions Modulate Gel Network Properties for Controlled Delivery

*Iulia Matei, Alexandra Busuioc, Ludmila Aricov, Anca-Ruxandra Leontieș, Vlad Tudor Popa, Aurica Precupas**
“Ilie Murgulescu” Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
Corresponding author: aprecupas@icf.ro

The potential of zein gels as functional delivery platforms for resveratrol (RESV), a natural polyphenol with anti-amyloid properties but low bioavailability, is systematically explored through a multi-methodological approach. This study combines spectroscopic (circular dichroism, infrared, fluorescence, UV–Vis), calorimetric (differential scanning microcalorimetry), and rheological methods with molecular docking to map the interaction sites, driving forces and structural changes from a soluble protein–polyphenol system to a three-dimensional gel network. Spectroscopic and molecular docking analyses reveal that the sol–gel transition is governed by hydrophobic forces and hydrogen bonding between RESV and the protein native structure. The polyphenol modulates zein structural and thermal stability in a concentration-dependent manner. In solution, RESV acts as a promoter of zein aggregation, with a higher effect at a RESV:zein 1:1 molar ratio. RESV induces conformational changes in the protein structure that influence the gelation of the protein. RESV:zein 4:1 molar ratio disrupts intermolecular associations, causing significant viscoelastic deformation and lower rheological moduli. In contrast, the RESV:zein 1:1 gel network demonstrates optimal viscoelastic properties. These structural and mechanical properties influence the functional release kinetics of the polyphenol. The release profile of RESV from zein gels in aqueous buffer demonstrates a distinctive bi-phasic transition, moving from an initial rapid diffusion to a prolonged, matrix-controlled release phase driven by the compaction of the hydrophobic zein matrix. Because zein maintains native structural resistance in gastric environments but is highly susceptible to pancreatin digestion, these matrices represent promising candidates for oral delivery. Therefore, these findings may contribute to the rational design of biopolymer-based encapsulation platforms modified to enhance bioavailability and optimize the gastrointestinal delivery of hydrophobic bioactive compounds.

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P2.25 Stochastic Electrochemical Sensor Based on Poly-erythrosine B/TiO_2@S-doped Graphene for Enantioselective Detection of L- and D-Citrulline

*Ionela Raluca Comnea-Stancu[1], Ramona Georgescu-State[1], Damaris-Cristina Gheorghe[1], Catalina Cioates Negut[1], Cristina Surdu-Bob[2], Raluca-Ioana Stefan-van Staden[1], Ruxandra-Maria Ilie-Mihai[1]**
1. Laboratory of Electrochemistry and PATLAB, National Institute of Research and Development for Electrochemistry and Condensed Matter, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Low Temperature Plasma Laboratory, National Institute for Lasers, Plasma and Radiation Physics (NILPRP), 409 Atomistilor St., 077125 Magurele, Romania

Poly-erythrosine B functionalised TiO_2@Sulfur doped graphene (polyERY/TiO_2@S-Gr) was employed to develop a novel stochastic electrochemical sensor that is capable of selectively detecting L and D-citrulline. The consistent integration of polyERY and TiO_2@S-Gr onto the single-walled carbon nanotube screen printed electrode (SWCNTPE) was validated by structural and morphological investigations, which enhanced the efficacy of molecular recognition and electron transfer kinetics. The electrochemical properties of the fabricated interfaces were evaluated using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), demonstrating enhanced charge-transfer capabilities and a larger electroactive surface area. The sensing interface exhibited minimal limitations of

quantification, broad linear concentration ranges, and remarkable sensitivity, enabling the concurrent detection of both enantiomeric forms of citrulline in complex biological matrices, including whole blood and saliva. This work introduces a sustainable, selective, and high-performance stochastic interface for the enantioselective detection of citrulline in biological and clinical research. The sensing interface demonstrated negligible quantification constraints, extensive linear concentration ranges, and exceptional sensitivity, facilitating the simultaneous identification of both enantiomeric forms of citrulline in intricate biological matrices such as whole blood and saliva.

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P2.26 Stochastic Electrochemical Detection of IL-6 and IL-8 Using a Green-Engineered AgNSs/CeO_2NPs–rGO@Pd Nanocomposite

Ramona Georgescu-State[1], Ionela Raluca Comnea-Stancu[1], Damaris-Cristina Gheorghe[1], Catalina Cioates Negut[1], Raluca-Ioana Stefan-van Staden[1], Marius Badulescu[2], Ruxandra-Maria Ilie-Mihai[1]
1. Laboratory of Electrochemistry and PATLAB, National Institute of Research and Development for Electrochemistry and Condensed Matter, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Low Temperature Plasma Laboratory, National Institute for Lasers, Plasma and Radiation Physics (NILPRP), 409 Atomistilor St., 077125 Magurele, Romania

A green-engineered stochastic electrochemical platform was developed for the sensitive and selective detection of the pro-inflammatory cytokines IL-6 and IL-8 using an AgNSs/CeO_2NPs–rGO@Pd nanocomposite-modified screen-printed carbon electrode. The sensing interface combines the catalytic and electroactive properties of the hybrid nanocomposite with the advantages of stochastic electrochemical recognition. CeO_2 nanoparticles were prepared through a sustainable synthesis route employing tea extract, providing an environmentally friendly alternative to conventional chemical synthesis. The modified electrode exhibited improved charge-transfer characteristics and enhanced electroactive surface area, resulting in highly sensitive analytical responses. Wide linear concentration ranges were obtained, from 4.00×10^{-18} to 1.00×10^{-6} g mL^{-1} for IL-6 and from 1.00×10^{-20} to 1.00×10^{-6} g mL^{-1} for IL-8, with ultralow quantification limits. The proposed approach enabled the determination of both cytokines in complex biological matrices, including tumor tissue, urine, whole blood, and saliva. Recoveries above 98% and relative standard deviations below 0.2% demonstrated the accuracy and reproducibility of the measurements. The combination of green nanomaterial synthesis, stochastic electrochemical detection, and a miniaturized electrode architecture highlights the potential of the proposed platform for ultrasensitive analysis of clinically relevant biomarkers in complex biological samples.

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P2.27 Anatomical and Micromorphological Characterization of Malus sylvestris (L.) Mill. Leaves from Telega, Romania, Using Light and Scanning Electron Microscopy

Cristina-Silvia Stoicescu[1], Cornel Munteanu[1], Robert Ancuceanu[2], Mihaela Dinu[2], Marilena-Viorica Hovanet[2], Adriana-Iuliana Anghel[2]**
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Department of Pharmaceutical Botany and Cell Biology, "Carol Davila" University of Medicine and Pharmacy, Traian Vuia 6, Bucharest, Romania
Corresponding authors: cristina.silvia.stoicescu@gmail.com, adriana.anghel@umfcd.ro

Introduction and aim: Malus sylvestris (L.) Mill. (Rosaceae), European wild apple, is a woody species native to Europe. The anatomical and micromorphological characteristics of the leaves, such as stomata, non-glandular trichomes, the cuticle, and cuticular waxes, enable the identification of plant products derived from this species and provide reference information for future studies.
Material and methods: Archived light microscopy and SEM micrographs of Malus sylvestris (L.) Mill. leaves collected in May–June from Telega, Romania, were qualitatively re-examined. The fresh material was identified, shade-dried under ventilated conditions, and stored under laboratory conditions. For light microscopy, cross-sections of the leaf blade, midrib, and petiole were cleared with sodium hypochlorite, double-stained with iodine green and alum carmine, and examined using a Nikon Labophot 2 microscope; surface preparations cleared with 5% NaOH or KOH were also assessed. For SEM, specimens mounted on double-sided carbon tape were examined using a Quanta 3D FEG microscope at 5 kV under high-vacuum conditions with an Everhart–Thornley detector.
Results and Discussion: Cross-sections showed a dorsiventral leaf blade with two palisade layers and spongy parenchyma containing calcium oxalate druses, particularly near the midrib. The midrib displayed subepidermal

angular collenchyma, druse-bearing ground parenchyma, and a collateral vascular bundle surrounded by a collenchymatous pericycle; the petiole contained one large central and two smaller lateral bundles, non-glandular trichomes, and druses.
SEM revealed navicular anomocytic stomata restricted to the abaxial epidermis and long, unicellular non-glandular trichomes with ribbon-like or cylindrical morphologies on both surfaces, more abundant abaxially and along the veins. Cuticular striations were more evident abaxially, whereas crystalliform epicuticular wax aggregates occurred adaxially. Together, these observations support the pharmacognostic characterization of the plant material.
Conclusions: Light and SEM provided complementary information on the internal anatomy and surface micromorphology of Malus sylvestris (L.) Mill. leaves. The combined anatomical and epidermal traits support the pharmacognostic characterization of the plant material. These descriptive findings provide a basis for future quantitative studies and comparisons among samples from contrasting ecological conditions.

P2.28 Spin Probe Behaviors in DES Systems

Florentina D. Vasile, Alexandru-Gabriel Bucur, Sevasti Matsia, Gabriela Ionita
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

Deep eutectic solvents (DESs) are low-melting liquid systems generally obtained by combining a hydrogen-bond acceptor (HBA) with a hydrogen-bond donor (HBD). The formation of an extended network of hydrogen-bonding and other intermolecular interactions results in a strong depression of the melting point and gives rise to physicochemical properties that can be tuned by changing the nature and ratio of the components. DESs have attracted increasing interest as alternative solvent systems due to their low volatility, relatively low cost, ease of preparation and, depending on their composition, favorable environmental characteristics. Their preparation is generally straightforward and involve simple heating and stirring of the components until a homogeneous liquid is formed. Choline chloride (ChCl) represents one of the most widely used HBA components in DES formulations, allowing the preparation of systems with different hydrogen-bond donors and compositions.
In this work, we aimed to investigate the behavior of spin probes in DES matrices by electron paramagnetic resonance (EPR) spectroscopy, using choline chloride-based systems with various HBD and allowing different DES compositions to be explored. The objective was to determine how the molecular environment and dynamics experienced by the spin probe were affected by the specific organization of the DES matrix. The EPR spectra were analyzed by spectral simulation, with particular attention to the g-tensor, nitrogen hyperfine coupling constant (AN), intrinsic linewidth (lwpp) and rotational correlation time (τ_{corr}), together with the relative contribution of different spectral species.
The influence of DES composition, HBA:HBD ratio was considered in order to establish their relationship with the local environment and dynamics of the spin probe. Ultimately, we aimed to correlate the changes observed in the EPR spectral parameters with the molecular organization and physicochemical properties of the DES matrix, providing insight into how spin probes could be used to characterize the microenvironment, intermolecular interactions and dynamics of DES systems.

Poster Session 3

Day 3 — Thursday, 25 September · 10:00 – 15:00 (Solution Showcase & Interactive Discussions — Startups • Industry • ANSO Representatives, ROMPHYSCHEM 18th edition)

Sustainable Innovation & Circular Economy

P3.01 Silica Aerogels for Environmental Applications

*George-Alin Balan[1,2], Andreea Luiza Mirt[1,3], Ludmila Motelica[3,4], Roxana Doina Trusca[1,3], Denisa Ficai[3-6], Ovidiu Cristian Oprea[3-6], Anton Ficai[1,3,4,6]**

1. Department of Science and Engineering of Oxide Materials and Nanomaterials, National University of Science and Technology Politehnica Bucharest, 011061 Bucharest, Romania
2. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
3 National Centre for Micro- and Nanomaterials, National University of Science and Technology Politehnica Bucharest, 060042 Bucharest, Romania
4. Research Center for Advanced Materials, Products and Processes, National University of Science and Technology Politehnica Bucharest, 060042 Bucharest, Romania
5. Department of Inorganic Chemistry, Physical Chemistry and Electrochemistry, Faculty of Applied Chemistry and Materials Science, University POLITEHNICA of Bucharest, 011061 Bucharest, Romania
6. Academy of Romanian Scientists, 050045 Bucharest, Romania

Water pollution from synthetic dyes discharged by the textile, cosmetic, pharmaceutical and food industries remains a major environmental concern, as these compounds are toxic and poorly biodegradable. Nanostructured silica aerogels, with their high specific surface area, high porosity and low density, are promising adsorbents for environmental remediation of dye-contaminated water. Silica aerogels were synthesized by the sol-gel method and characterized by FTIR, TG-DSC, BET and SEM. FTIR confirmed the Si-O-Si silica network and surface silanol groups, while BET analysis showed a specific surface area of 677.2 m^2/g, a pore volume of 0.6753 cm^3/g and an average pore diameter of 3.989 nm. SEM revealed a hierarchical, fragile porous morphology of near-spherical nanoparticles, and the aerogel reached a dynamic swelling ratio of 73.92% in water. The environmental applicability was evaluated through selective adsorption of methylene blue (MB, cationic) and methyl orange (MO, anionic), monitored by UV-Vis spectroscopy. The unmodified aerogel selectively adsorbed MB, reaching an equilibrium capacity of 45.16 mg/g, while MO adsorption remained negligible, confirming the dominant role of electrostatic interactions between the negatively charged surface and the dye molecules. These results highlight sol-gel silica aerogels as selective, low-cost adsorbents for environmental water-treatment applications.

P3.02 Solar-Simulated Photocatalytic Removal of the Anti-Cancer Drug Epirubicin in the Presence of LDH-Based Co_3Fe Systems and Derived Oxides

*Dragoș-Sebastian Baltag[1], Adina Răducan[1], Petruța Oancea[1], Bogdan Cojocaru[1,2], Rodica Zăvoianu[1,2], Vasile I. Pârvulescu[1,2], Octavian D. Pavel[1,2]**

1. University of Bucharest, Faculty of Chemistry, 4-12 Regina Elisabeta Blv, 030018 Bucharest, Romania
2. Research Center for Catalysts & Catalytic Processes, Faculty of Chemistry, University of Bucharest, 4-12 Regina Elisabeta Blv., 030018 Bucharest, Romania
Corresponding author: octavian.pavel@chimie.unibuc.ro

Global efforts to improve living standards and life expectancy have increased industrial and municipal activities, generating significant chemical waste. Persistent contaminants like synthetic dyes and pharmaceuticals in municipal wastewater resist conventional treatments, posing risks to ecosystems and human health and necessitating improved remediation methods.

Advanced Oxidation Processes (AOPs), especially photocatalysis, offer effective degradation by producing reactive species such as hydroxyl radicals that break down complex pollutants under mild conditions without secondary pollution. Integrating AOPs into wastewater treatment can substantially reduce hazardous residues, supporting sustainable water management.

Our research is focused on the development of tailored photocatalytic systems based on layered microscopic materials synthesized via a conventional co-precipitation (CP) method, together with mixed oxides obtained through thermal treatment in air. The investigated materials are derived from low-cost transition metal ions, namely Co^{2+} and Fe^{3+}, and were synthesized using either organic (tetramethylammonium hydroxide, TMAH) or inorganic hydrolysis agents (NaOH / Na_2CO_3), while maintaining a constant M^{2+}/M^{3+} molar ratio of 3. Comprehensive physicochemical characterization by XRD, DRIFTS, ATR and DR-UV-Vis confirmed the formation of layered and oxide phases, which are responsible for the observed photocatalytic performance.

To evaluate the photocatalytic properties of these materials, the anti-cancer drug Epirubicin was used as a degradation-target pollutant, utilizing sunlight simulated by an LED lamp (35 klx). Photocatalyst concentration varied

between 0.33-1.33 mg/mL, and Epirubicin concentration ranged from 2.5-4×10^{-4} M. The degree of discoloration of the solution was assessed by measuring the variation in absorbance of the pollutant solutions using a Jasco Carry 50 spectrophotometer.
The most effective results, η = 95.66%, were achieved for simulated-solar 4×10^{-4} Epirubicin degradation using 1 mg/mL LDH Co3Fe IA CP in 80 minutes. The oxide microscopic materials obtained from the LDH precursor manifested smaller photocatalytic efficiency. Additionally, for the best catalyst, an adsorption study was conducted.

P3.03 Green Corrosion Protection Using Aqueous Spent Coffee Grounds Extract

Florina Branzoi[1], Elena Ionela Neacsu[1], Marius Alexandru Mihai[1], Iulia Harabor[2]*
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. National College "Virgil Madgearu"
Corresponding author: fbrinzoi@chimfiz.icf.ro

This study evaluates the corrosion inhibition performance of green inhibitors obtained from spent coffee grounds (SCGs) for brass in 0.5 M H_2SO_4 and 1 M HCl solutions. The aqueous SCG extracts were prepared using optimized extraction procedures and characterized by HPLC analysis. Their corrosion protection efficiency was assessed by potentiodynamic polarization and electrochemical impedance spectroscopy (EIS). FT-IR spectroscopy and SEM-EDX analyses provided evidence for the formation of a protective film on the brass surface, which was attributed to the adsorption of organic constituents present in the SCG extracts. The adsorption process was found to follow the Langmuir isotherm, with high adsorption equilibrium constants and negative values of ΔG°ads, indicating a spontaneous adsorption process involving both physisorption and chemisorption. Thermodynamic investigations performed over the temperature range of 293–333 K further demonstrated the temperature dependence of the inhibition process. Notably, inhibitors exhibited excellent corrosion inhibition performance at concentrations of 800 and 1000 ppm, achieving inhibition efficiencies of up to 96% (1 M HCl) and 95% 0.5 M H_2SO_4).

P3.04 Natural Origin Hydrogels Based on Green Tea Extract with ROS Scavenging Feature for Skin Wound Healing

Mariana Chelu[1], Monica Popa[1], Laura Mihaela Stefan[2], Ana-Maria Seciu-Grama[2], Andreea Plangu[2], Jose María Calderon Moreno[1]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Department of Cellular and Molecular Biology, National Institute of Research and Development for Biological Sciences, 296 SplaiulIndependentei, Bucharest 060031, Romania

Multifunctional hydrogels incorporating natural bioactive compounds offer promising opportunities for biomedical and skincare applications. In this study, two composite hydrogels based on Aloe vera gel were formulated and characterized, one formulation of which was enriched with green tea extract. Pharmacotechnical, physicochemical, and biological properties were evaluated, including pH, viscosity, consistency, spreadability, moisture retention, swelling behavior, and cellular responses. Both hydrogels were homogeneous and exhibited suitable physicochemical characteristics. Green tea extract improved moisture retention, increased the swelling ratio by approximately 150%, and enhanced structural stability. Both formulations showed good cell compatibility below 50 mg/mL, promoted cell proliferation and migration, and reduced oxidative stress. These results demonstrate the potential of polyphenol-rich botanical extracts to improve the functional and structural properties of Aloe vera-based hydrogels for moisturizing and skin-care applications.

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P3.05 Solar-Active Photocatalytic Beads for Organic Pollutants Removal

Maria Covei, Ioana Tismanar [1], Cristina Bogatu[1], Jose Maria Calderon Moreno[2], Irina Atkinson[2], Veronica Bratan[2], Mariuca Gartner[2]
1. Transilvania University of Brasov, RESREC, Romania
2. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

Advanced wastewater treatment technologies are increasingly required to remove trace organic pollutants that remain in treated wastewater at ppm or ppb concentrations and may limit its safe reuse. Heterogeneous photocatalysis represents a promising wastewater treatment approach. However, practical implementation is constrained by the configuration of the photocatalyst. Suspended powders have a high surface area but require

catalyst recovery, while immobilized thin films facilitate separation and handling but offer a lower available surface area.
In this study, a TiO_2–g-C_3N_4 composite was immobilized as thin films on 2 mm glass beads to investigate a configuration that combines easy catalyst recovery with the geometrical surface-area advantage provided by small spherical supports. The use of 2 mm beads provides an approximately 3.6-fold theoretical increase in geometrical surface area compared to a planar substrate occupying the same projected area.
The TiO_2–g-C_3N_4 composite was prepared by the sol-gel method using a TiO_2 seeding layer followed by a second layer containing 5 wt.% g-C_3N_4. XRD analysis confirmed the formation of anatase, while XRF, EDX, and Raman analyses provided evidence consistent with the presence of g-C_3N_4-related species in the composite coating. SEM analysis revealed continuous coatings characterized by surface aggregates.
Photocatalytic activity was evaluated using methylene blue and imidacloprid as model pollutants in a custom-designed 0.6 L recirculating continuous-flow photoreactor operated at 2 L min^{-1} under natural solar irradiation (G_{tot} = 550 W m^{-2}, G_{uv} = 10 W m^{-2}). Using 6 g of coated beads per 1 L of 10 ppm pollutant solution, degradation efficiencies of approximately 50% for methylene blue and 40% for imidacloprid were obtained after 8 h. The results demonstrate the feasibility of the proposed configuration for solar-driven photocatalytic treatment under recirculating continuous-flow conditions. Further studies addressing long-term cycling, mineralization, degradation intermediates, charge-transfer mechanisms and performance in real wastewater are required to assess its practical applicability.

P3.06 Thermochemical Performance of Biomass Pellets for Sustainable Energy

*Ana Neacsu, Daniela Gheorghe**
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Laboratory of Chemical Thermodynamics,202 SplaiulIndependentei, 060021 Bucharest, Romania
Corresponding author: dgheorghe@icf.ro

Biomass residues represent an important renewable resource for sustainable energy production and waste valorization. However, their direct use as solid fuels can be limited by variable moisture content, low bulk density and differences in chemical composition and ash content. These characteristics influence fuel handling, storage, transportation, and combustion behavior, highlighting the need for suitable biomass upgrading strategies. Pelletization is an effective densification approach that converts loose biomass residues into compact and more homogeneous solid fuels with improved handling and storage characteristics. The properties of the resulting pellets depend strongly on the characteristics of the raw biomass and on the use of different biomass blends.
Among the parameters used to evaluate the energy performance of solid biomass fuels, the gross calorific value (GCV), or higher heating value (HHV), is of particular importance because it represents the total heat released during complete combustion. The lower heating value (LHV), which excludes the latent heat associated with water vaporization, provides an estimate of the net energy available under practical combustion conditions. Therefore, the combined assessment of GCV/HHV and LHV, together with relevant physical and chemical properties, provides a reliable basis for evaluating the fuel quality and energy potential of biomass pellets.
In the present study, biomass pellets produced from selected feedstocks, agro industrial residues both individually and as biomass blends, were investigated to assess the relationships between their physicochemical characteristics and calorific performance. The GCV/HHV was experimentally determined using a Parr 6200 oxygen bomb calorimeter, while the corresponding LHV was calculated. Moisture content and bulk density were determined as relevant physical fuel properties, whereas ash content was evaluated after combustion. The results provide an integrated evaluation of the factors influencing the calorific properties of biomass pellets and highlight the potential of biomass blending for improving their energy characteristics.

P3.07 Radiation-Grafted Ground Tire Rubber as a Novel Adsorbent for Copper Ion Removal from Water

Lorant Kiss[1], Renata Homlok[2], Petra Toth[1], Anna Tegze[2], Laszlo Meszaros[1,3]
1. Department of Polymer Engineering, Faculty of Mechanical Engineering, Budapest University of Technology and Economics, Muegyetemrkp. 3, Budapest H-1111, Hungary
2. Radiation Chemistry Group, Surface Chemistry and Catalysis Department, Institute for Energy Security and Environmental Safety, HUN-REN Centre for Energy Research, Konkoly-Thege M. Street 29-33, Budapest H-1121, Hungary
3. HUN-REN-BME Research Group for Composite Science and Technology, Budapest University of Technology and Economics, Muegyetemrkp. 3, Budapest H-1111, Hungary

Heavy metal contamination of water resources, for instance by copper ions, poses a serious environmental and public health concern due to their toxicity and non-biodegradable nature. Conventional removal methods are often costly, which has increased interest in low-cost adsorbents made from waste materials. Ground tire rubber (GTR), produced by grinding end-of-life tires, is an abundant and has potential as a cost-effective adsorbent. However, its non-polar surface with low functional group density typically limits its adsorption capacity in untreated form.
In this study, radiation-induced grafting was used to introduce functional monomers onto the GTR surface to enhance its affinity for copper ions. Samples were irradiated using a TESLA LINAC LPR-4 electron accelerator (4 MeV), both in

air and in a water medium, to compare the effect of the irradiation medium on grafting efficiency. The irradiated GTR was then grafted with methyl methacrylate (MMA, undiluted) or maleic anhydride (MAH, 10 wt% in acetone) at 50 °C. FTIR and SEM analyses of the resulting materials (GTR-g-MMA and GTR-g-MAH) confirmed the formation of oxygen-containing functional groups and distinct changes in surface morphology.
Copper-ion adsorption performance was evaluated through batch experiments examining the effects of initial concentration, contact time, pH, and absorbed dose. Radiation grafting significantly improved copper adsorption capacity compared to untreated GTR, confirming the successful introduction of metal-binding functional groups. These findings highlight radiation-grafted ground tire rubber as a novel, low-cost, and environmentally friendly adsorbent for copper removal from water, offering an effective route for both waste tire valorization and water treatment.

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P3.08 Degradation of Phenol in Aqueous Solution Using Electron Beam Irradiation and Ozone: Towards a Combined Treatment Approach

Renáta Homlok[1], Anna Tegze[1], Monica Pavel[2], Erzsébet Takács[1], László Wojnárovits[1], Krisztina Kovács[1]
1. Radiation Chemistry Group, Surface Chemistry and Catalysis Department, Institute for Energy Security and Environmental Safety, HUN-REN Centre for Energy Research, Konkoly-Thege Miklós út 29–33, 1121 Budapest, Hungary
2. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

Phenol is a widely used industrial chemical and a frequently detected contaminant in effluents originating from petrochemical, pharmaceutical, and resin manufacturing processes. Due to its toxicity and limited removal by conventional biological treatment, its effective elimination from aqueous matrices remains a significant environmental challenge. Advanced Oxidation Processes (AOPs), based on the generation of highly reactive species such as hydroxyl radicals (•OH), offer a promising approach for the degradation of persistent organic pollutants.
In this study, the degradation of phenol in aqueous solution was investigated using two advanced oxidation approaches: electron beam (e-beam) irradiation and ozone treatment. Aqueous phenol solutions with an initial concentration of 20 mg/L were treated using different absorbed doses of electron beam irradiation and, separately, under controlled ozone treatment conditions. A newly established ozone treatment system was tested for its applicability to phenol degradation. The effects of the treatments were evaluated by monitoring changes in UV absorbance, pH, chemical oxygen demand (COD), and total organic carbon (TOC).
Under air-saturated conditions, electron beam irradiation effectively degraded phenol through reactions initiated by the reactive species primarily hydroxyl radicals generated during water radiolysis. Ozone treatment also promoted phenol degradation, demonstrating the applicability of the newly established ozonation system for the treatment of phenol-containing aqueous solutions. Changes in UV absorbance, COD, and TOC, together with phenol removal, were used to assess the extent of oxidation and degradation during the treatments.
The comparison of the two individual treatment approaches provides a baseline assessment of their respective degradation efficiencies and operating requirements. The results obtained in this study establish an experimental basis for the future development of a combined e-beam/O_3 treatment process, in which the potential complementary effects of radiolytic and ozonation reactions can be investigated. The present work therefore represents an initial step towards the development of an integrated e-beam–ozone advanced oxidation process for the treatment of phenol-containing wastewater.

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P3.09 Salt Induced Activation of Trametes Versicolor Laccase for Textile Dye Degradation

Anca-Ruxandra Leontieș, Raluca-Marieta Toma, Adina Răducan, Gabriela Stîngă, Monica Elisabeta Maxim, Adriana Băran, Lumila Aricov*
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania

Fungal laccase (Lc) has gained significant attention in biotechnology because it can effectively oxidize various toxic wastewater contaminants, such as synthetic dyes, pesticides, and pharmaceuticals. There are a number of drawbacks associated with the use of laccases for the biodegradation of aqueous pollutants. These drawbacks include high production costs, limited activity under severe environmental conditions, susceptibility to proteolysis, and inactivation. As a result, the Lc treatment is not economically practical. To mitigate unwanted side effects, activity modulators can be used to control enzyme performance. Here, we applied sodium sulfate to regulate laccase (Lc)

activity during naphthol green (NG) degradation. Chosen for its prevalence in textile wastewater, the salt serves as a non-essential activator. In the presence of sodium sulfate, NG decomposition conformed to Michaelis-Menten kinetics, with the salt acting as a non-essential activator. This activation significantly enhanced enzymatic activity through a nonlinear, concentration-dependent mechanism.

P3.10 Energy Valorization of Biomass Waste: Hydrothermal Carbonization of Orange Peels

Ana Neacsu[1], Ancuta Mihaela Sofronia[1], Daniela Gheorghe[1], Oana Nicoleta Nicula[2], Ioana Ion[2]**

1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. National Institute for Research and Development in Electrical Engineering ICPE-CA Bucharest (ICPE-CA), 313 Spl. Unirii, 030138, Bucharest, Romania

Corresponding authors: amsofronia@yahoo.com, ion.ioana@icpe-ca.ro

This paper presents preliminary results on the energetic valorization of orange peel waste for use in combustion applications. The proposed methodology utilizes hydrothermal carbonization to convert wet biomass (HHV 16.26 MJ/kg) into hydrochar, a material with high energy density (HHV 22 MJ/kg). This technological approach transforms a waste product—which, through natural decomposition, would pollute soil and water and generate greenhouse gases—into a sustainable solid fuel with a low carbon footprint. Unlike classic pyrolysis (which requires dry biomass with less than 10% moisture), hydrothermal carbonization is efficient for raw materials with up to 90% moisture, with its primary advantage being the elimination of the need for energy-costly preliminary drying.

P3.11 Enhanced Paracetamol Degradation by Catalytic Ozonation over Pd-Decorated Ce–$SrTiO_3$ and $SrTiO_3$ Catalysts

Irina Atkinson[1], Gabriela Petcu[1], Mihaela-Alina Oprea[2], Maria-Carina Carabulea[2], Ionuț-Alexandru Colțănel[2], Ciprian Ghenghea[3], Ioana Alexia Radu[4], Gabriela Stîngă[1], Monica Elisabeta Maxim[1], Adriana Băran[1], Florica Papa[1]

1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. National University of Science and Technology POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnologies, Gheorghe Polizu 1-7, 011061 Bucharest, Romania
3. National University of Science and Technology POLITEHNICA Bucharest, Faculty of Materials Science and Engineering, Spl. Independenței 313, 060042 Bucharest, Romania
4. International Computer High School of Bucharest, Balta Albina 9, 032622 Bucharest, Romania

Paracetamol is frequently detected in wastewater and natural aquatic environments because of its extensive use and incomplete removal during conventional wastewater treatment. To address this challenge, Pd-decorated Ce–$SrTiO_3$ and $SrTiO_3$ catalysts were synthesized for the catalytic ozonation of paracetamol in aqueous solution. The perovskite supports were prepared using the Pechini sol–gel method, while Pd nanoparticles were synthesized via an alkaline polyol route and subsequently deposited onto the calcined perovskites. Thermal treatment of the precursor perovskite gel was selected based on differential thermal analysis/thermogravimetric (DTA/TG) analysis, and the size of the Pd nanoparticles was determined by dynamic light scattering (DLS). The resulting catalysts were characterized by X-ray diffraction (XRD), H_2 temperature-programmed reduction (H_2-TPR), UV–Vis spectroscopy, scanning electron microscopy (SEM), and H_2 chemisorption. Catalytic performance was evaluated for the ozonation of paracetamol at a catalyst loading of 0.5 g L^{-1}, and the paracetamol degradation was monitored by UV–Vis spectroscopy. Both Pd-decorated Ce–SrTiO3 and SrTiO3 exhibited outstanding performance, achieving complete paracetamol degradation within 30 minutes. These results highlight the potential of Pd-modified Ce–$SrTiO_3$ and $SrTiO_3$ perovskites as efficient catalysts to remove persistent pharmaceutical pollutants from water.

P3.12 Structure-Dependent Photocatalytic Degradation of Phenol: A Parallel Assessment of Layered Perovskites and Calcined Layered Double Hydroxides

Monica Pavel[1], Crina Anastasescu[1], Anca Vasile[1], Renata Homlok[2], Anna Tegze[2], Krisztina Kovacs[2], Irina Atkinson[1], Florica Papa[1], Liubovi Cretu[1], Razvan State[1], Ioan Balint[1]

1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Radiation Chemistry Group, Surface Chemistry and Catalysis Department, Institute for Energy Security and Environmental Safety, HUN-REN Centre for Energy Research, Konkoly-Thege Miklós út 29-33, 1121 Budapest, Hungary

Solar-driven catalysis offers a highly sustainable strategy to mitigate global challenges, including clean hydrogen generation, CO2 reduction, and environmental remediation. Layered architectures offer promising advantages in light-related applications due to unique physicochemical characteristics that surpass those of conventional materials. The electronic and structural properties of Dion-Jacobson-type layered perovskites can be adjusted through multiple modification methods, including ion exchange, a versatile approach for fabricating new layered assemblies. In parallel, layered double hydroxides (LDHs) serve as promising materials for energy-active applications owing to their large specific surface area, tunable compositions, and characteristic "memory effect".

This study focuses on two classes of layered compounds tailored for advanced oxidation processes: (*i*) layered perovskites (pristine $RbLaTa_2O_7$ and protonated $HLaTa_2O_7$), and (*ii*) calcined layered double hydroxides (ZnAl and CoAl LDHs). These compounds were structurally characterized using multiple techniques and evaluated for the photocatalytic degradation of phenol under simulated solar irradiation. The developed layered architectures demonstrated highly promising performance for environmental remediation applications.

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P3.13 Amino Acid-Functionalized Styrene-Divinylbenzene Copolymer for Environmental Remediation

Adriana Popa[1], Lavinia Lupa[2], Anca Filimon[3], Aurelia Visa[1]*
1. "Coriolan Drăgulescu" Institute of Chemistry, 24 Mihai Viteazul Blv., 300223 Timisoara, Romania
2. Politehnica University Timișoara, Faculty of Chemical Engineering, Biotechnology and Environmental Protection, 6 Vasile Parvan Blvd., 300223, Timisoara, Romania
3."Petru Poni" Institute of Macromolecular Chemistry, 41A Aleea Grigore Ghica Vodă, 700487 Iași, Romania
Corresponding author: apopa_ro@yahoo.com; apopa@acad-icht.tm.edu.ro

Growing environmental concerns and the increasing demand for efficient water treatment technologies have stimulated the development of functionalized polymeric materials for the removal of contaminants from water. Among them, styrene-divinylbenzene (S-DVB) copolymers are of particular interest due to their high chemical and mechanical stability, and their adsorption performance can be improved by introducing pendant functional groups. In this context, the present study extends previous research on S-DVB copolymers functionalized with nitrogen-containing derivatives by introducing amino acid functionalities, designed to increase the affinity of the material for metal ions.

Styrene-divinylbenzene copolymer supports were functionalized with amino acid groups using a phase-transfer catalysis-based strategy. The obtained material (S-12%DVB, denoted AM) was characterized by Fourier transform infrared spectroscopy (FTIR), energy dispersive X-ray spectroscopy (EDX), scanning electron microscopy (SEM) and thermogravimetric analysis (TGA), to confirm the successful incorporation of amino acid groups into the polymer network. The degree of functionalization was estimated by determining the fraction of repeating units containing pendant amino acid groups, based on the statistical structure proposed for the AM copolymer.

The introduction of amino acid groups provides the material with coordination centers containing nitrogen and oxygen atoms, capable of interacting with metal ions. Thus, the functionalized copolymer represents a promising adsorbent for water decontamination applications, especially for the removal of copper ions.

Therefore, this study evaluated the adsorption performance, regeneration potential, and practical applicability of S-DVB as an effective, reusable, and sustainable adsorbent for copper removal from aqueous systems, supporting the achievement of United Nations Sustainable Development Goal (UN SDG) 6, Target 6.3, by contributing to environmentally friendly water purification and trace metal remediation.

P3.14 Sea Water Effect on Different Natural Stones-A Laboratory Study

Ana-Maria Julieta Popescu[1], Mihai Anastasescu[1], Cosmin Codrea[1], Florin Ghita[2]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021 Bucharest, Romania
2. Rock Star Construct SRL (Piatraonline), 137 A Aleea Teisani, Bucharest

This work aimed to study the mechanism of alteration of different natural stones exposed to the marine environment. Each natural stone differs in chemical content, color, and texture. These differences in the characteristics of natural stones affect the degree of deterioration. We chose marble, travertine and limestone in this study, which are all calcareous stones. Since they have a similar chemical composition, they are very sensitive to saltwater environments. However, their structural and surface differences make them react to seawater in unique ways. We correlated the corrosion data with the surface data. The methods used were: weight loss measurements in artificial seawater, atomic force microscopy (AFM) and profilometry, to determine which of these natural stones are suitable for exterior building materials in marine environments.

P3.15 Crown Ether-Functionalized Hydrochars as Potential Adsorbents for Copper and Lead Ions from Water

Greta M. Patrinoiu[1], Adelina Ianculescu[2], Jose Calderon-Moreno[1], Adina M. Musuc[1], Sorin Avramescu[3], Mihaela Florea[4],Petre Ionita[5]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy,202SplaiulIndependentei, 060021 Bucharest, Romania
2. University "Politehnica" Bucharest, Gh. Polizu St. 1-7, 011061 Bucharest, Romania
3. Faculty of Animal Productions Engineering and Management, University of Agronomic Sciences and Veterinary Medicine of Bucharest, 59 MarastiBvd., 011464 Bucharest, Romania
4. National Institute for Materials Physics, Atomistilor 405A, Magurele, 077125 Bucharest, Romania
5. University of Bucharest, Faculty of Chemistry, Panduri 90, 050663 Bucharest, Romania

Human activities associated with rapid urbanization, industrialization and climate change have significantly impacted environmental integrity and biological safety in recent decades [1].
Frequently detected in aquatic environments at relatively high concentrations, heavy metals pollution has become a major concern for environmentalists [2].
Here, we report a general, one-step hydrothermal functionalization of sustainable hydrochars (HC) with 4'-aminobenzo-15-crown-5 ether (CE) using sucrose, starch, and fructose as carbon sources. The crown ether functionalization and materials integrity were successfully confirmed: pristine and functionalized hydrochars were characterized by various techniques (SEM, Raman spectroscopy, FTIR, thermal analysis and X-ray photoelectron spectroscopy).
Batch adsorption measurements for Cu^{2+} and Pb^{2+} removal from aqueous solutions demonstrated that the Freundlich isotherm provided the best fit, suggesting multilayer and heterogeneous adsorption. The study highlights the potential of crown ether-functionalized hydrochars as sustainable materials for mitigating water pollution [3].

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P3.16 Development of Silver-Doped and Threonine-Functionalized Hydroxyapatite from Biowaste: Structural Insights and Thermal Stability

*A. Botea-Petcu, D. Gheorghe, A. Neacsu, I. Atkinson, E.M. Anghel, C. Marinescu, A. Sofronia**
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021, Bucharest, Romania
Corresponding author: amsofronia@yahoo.com

This work presents the synthesis and characterization of biomaterials based on hydroxyapatite (HA) obtained from sustainable natural precursors (eggshells). The study comparatively examines three types of samples: pure HA, silver-doped HA (HA-Ag), and silver-doped HA surface-functionalized with the amino acid threonine (HA-Ag-Th). The integration of silver into the crystal lattice aims to introduce antimicrobial properties, while the use of threonine serves as a surface modifier to enhance bioactivity [1-3].
The structural, morphological, and surface modifications induced by doping and functionalization were investigated in detail using complementary techniques: BET, X-ray diffraction (XRD), FTIR spectroscopy, UV-Raman, DLS, and Zeta potential. The structural analyses revealed nanometric particle sizes for all analyzed samples, crystal lattice modifications determined by the silver ions, as well as specific interactions between threonine and the inorganic matrix [4].
The thermal behavior of the three systems was evaluated through high-temperature TG-DSC analyses. The results highlighted a remarkable thermal stability for the samples doped and synthesized in the presence of the amino acid, which is a critical parameter for their subsequent processing as bone substitutes. The synergistic properties of the HA-Ag-Th sample indicate a high potential for use in bone tissue engineering.

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P3.17 Electrochemical Regeneration of Platinum Nanoparticles-Modified Electrodes used for the Discoloration of Organic Dyes

Milica Țară-Lungă-Mihali[1], Anca Lascu[1], Ionela Fringu[1],*Camelia Epuran[2], Ionut Fratilescu[2], Anemona Mariana Cornea[1], Nicoleta Pleșu[1]
1. "CoriolanDragulescu" Institute of Chemistry, 24 Mihai Viteazu Ave,300223 Timisoara, Romania
2. ICAM-Advanced Environmental Research Institute, West University of Timisoara,Oituz Street 4, 300233 Timisoara, Romania
Corresponding author: milicamihali22@gmail.com

Electrochemical processes are a viable alternative in management and reduction of pollution. The electrochemical process offers some advantages (no need to separate the catalyst from the reaction mixture, possibility of controlling the process by adjusting the variable current and potential, easy to automate the process) and can be used complementary to other treatments as biological. Malachite green (MG) is a triphenylmethane compound used as a dye for materials such as silk, leather, and paper, in the fish industry as an anti-fungal agent. MG is a thermostable colorant and thus may not be easily degraded and can cause carcinogenic symptoms [1]. The present study investigates the electrochemical regeneration of an electrode consisting in silica hybrid in which Pt nanoparticles are embedded, impregnated with malachite green (SH-PtNPs-MG). The synthesis of the material is previously published and follows the same procedure as for fuchsine B [2]. The used SH-PtNPs-MG was drop casted on the Pt electrode surface. The desorbed MG from the used hybrid is oxidized at Pt electrodes in NaCl 3% aqueous media at applied potential of 1.3V for 40 min. The electrochemical treatment is commonly based on the elimination of pollutants on the anode surface, via production of OH•, or/and other oxidants such as chlorine, persulfate, etc. [3]. The Cl− is used to generate active chlorine oxidants (Cl_2, HOCl and OCl−). The electrochemical behavior of the modified electrode was evaluated by cyclic voltammetry. The results demonstrated that the platinum nanoparticles-modified electrode exhibited enhanced electrochemical activity toward the investigated dyes, leading to a significant decrease in color intensity. The improved performance was attributed to the catalytic and electron-transfer properties of the platinum nanoparticles layer, which facilitates the oxidation and/or reduction of dye molecules at the electrode surface. The calculated yield of discoloration gives a good value of ~88%.

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P3.18 Effect of Zn Doping on the pH-Triggered Release of Sodium Risedronate from Hydrothermally Synthesized Hydroxyapatite

*Alina Botea-Petcu[1], Ancuta Sofronia[1], Romica Sandu[1], Daniela Gheorghe[1], Ioana Silvia Hosu[2], Georgeta Ramona Ivan[2], Irina Atkinson[1], Florentina Maxim[1], Speranta Tanasescu[1], Florina Teodorescu[1]**
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202SplaiulIndependentei, 060021, Bucharest, Romania
2. National Institute for Research & Development in Chemistry and Petrochemistry, ICECHIM, SplaiulIndependentei202, 060021, Bucharest, Romania
Corresponding author: fteodorescu@icf.ro

Hydroxyapatite (HAP), due to its chemical and structural similarity to bone mineral, is an effective, biocompatible carrier for controlled drug delivery systems. Sodium risedronate is a bisphosphonate drug used in osteoporosis therapy. Here, the hydrothermally synthesized HAP and zinc-doped hydroxyapatite (HAP-Zn) shown pure apatite phase formation confirmed by X-ray diffraction (XRD) analysis. Partial replacement of Ca^{2+} by Zn^{2+} is known to provide additional antibacterial activity to hydroxyapatite structure and proved to reduce crystallite size (from 9.66 to 9.08 nm), to increase specific surface area (from 44.9 to 59.3 $m^2\ g^{-1}$) and surface reactivity. In this work, two pH-sensitive risedronate delivery systems based on HAP and HAP-Zn, impregnated with the drug, are described. The risedronate-loaded hydroxyapatite systems were characterized using scanning electron microscopy equipped with energy-dispersive X-ray spectroscopy (SEM-EDX), Fourier-transform infrared spectroscopy (FTIR), dynamic light scattering (DLS), and isothermal titration calorimetry (iTC). Additionally, UV–Vis spectroscopy was used to quantify drug loading capacities and the release profiles of sodium risedronate. The results evidenced a pH-dependent release, indicating the potential of Zn-doped hydroxyapatite as a smart delivery system for osteoporosis, Paget's disease and metastatic bone disease.

P3.19 Square-Like Zero-Dimensional Prussian Blue Analogues

Diana Visinescu[1], Maria-Gabriela Alexandru[2], Sergiu Shova[3], Francesc Lloret[4]
1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021, Bucharest, Romania
2. Department of Inorganic Chemistry, Physical Chemistry and Electrochemistry, Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 1-7 Gh. Polizu Street, 011061 Bucharest, Romania

3. “Petru Poni” Institute of Macromolecular Chemistry, Romanian Academy, Aleea Grigore Ghica Vodă 41-A, RO-700487 Iaşi, Romania
4. Departament de QuímicaInorgànica, Instituto de Ciencia Molecular (ICMol), Universitat de València, 46980 Paterna, Valencia, Spain

Prussian Blue analogues (PBAs), with a cubic three-dimensional structure, are the oldest known metal-organic frameworks, exhibiting multifunctionality across different applications such as pigments, cyanotypes, ion exchangers, biosensing, or energy storage materials. Specifically, PBAs have made history in the field of molecular magnetism by providing the first examples of high-Tc molecular magnets and photomagnets.The strong interest in thoroughly investigating the magnetic exchange interactions in PBAs has stimulated the design and synthesis of model compounds. For example, zero-dimensional (0-D) PBAs with regular shapes, such as molecular squares, mimic the magnetic properties of a single face of a 3-D PBA and allow for straightforward theoretical modeling of magnetic data. Moreover, the square-like 0-D PBAs can exhibit new and intriguing magnetic properties such as slow magnetization relaxation (SMR) and single-molecule magnet behaviour. In this regard, cyano-bridged 3d–4f square-like molecules have emerged in recent years as new models for PBAs, incorporating key Ln(III) features, such as strong magnetic anisotropy and a high-spin ground state that further could trigger SMR. The most efficient approach to obtain cyano-bridged mixed 3d–4f squares relies on the simultaneous employment of two structural control elements: heteroleptictricyanometallates as bis-monodentate angular connectors, and auxiliary bidentate blocking ligands (e.g., chelating pyridine-derived ligands) capped on the coordination sites of Ln(III) ions to prevent polymerization. Herein, we describe the synthesis and magneto-structural characterization of a new series of cyano-bridged tetranuclear complexes in which Fe(III) and Ln(III) centers are alternatively arranged in the corners of a square. The static and dynamic magnetic properties, as well as the magnetocaloric properties of these cyano-bridged 3d–4f square-shaped heterometallic complexes, were investigated to determine the influence of the Ln(III) ion's nature on the spin dynamics and thermodynamics of the resulting complexes.

P3.20 Labels Containing AuAg Alloy Nanoparticles Encapsulated in Functionalized Silica for Lateral Flow Immunoassays

Iulia Ș. Voicu[1], Alin G. Gheorghe[1], Mihaela Deaconu[1,2], Bogdan Ș. Vasile[3], Cristian Matei[1], Daniela Berger[1]**
1. Department of Inorganic Chemistry, Physical Chemistry & Electrochemistry, National University of Science and Technology Politehnica Bucharest, 1-7 Polizu street, 011061, Romania
2. CAMPUS Research Institute, National University of Science and Technology Politehnica Bucharest, ROMANIA
3. Research Center for Advanced Materials, Products and Processes, National University of Science and Technology Politehnica Bucharest, 060042, Bucharest, ROMANIA
Corresponding authors: iulia.voicu1907@stud.chimie.upb.ro,daniela.berger@upb.ro

In recent years, the Lateral Flow Immunoassay (LFIA) gained reputation as a very attractive clinical tool, that performs as a ”lab-in-a-hand”, being an easy to use, cost-effective and time saving analytical method. It is widely used for the detection of molecules, microorganisms, markers and biomarkers in clinical tests [1]. However, sensitivity is the main concern regarding this kind of analysis, low limits of detection being required for medical tests. To overcome this issue, one can use labels, such as Au, or AuAg alloy nanoparticles, that can be conjugated with biomolecules [2].
AuAg alloy nanoparticles (NPs) were synthesized in an inert atmosphere using oleylamine as a reducing agent at 120 °C. The surface plasmon resonance of the AuAg nanoparticles can be tuned by modifying the synthesis conditions, hence achieving different Au/Ag ratios within the alloy. Then AuAg nanoparticles were incorporated with high yield in functionalized silica with 3-aminopropil and 3-mercaptopropil groups. The next step involved coating the resulting NPs with a hydrophob silica layer, followed by the application of an additional layer of silica functionalized with carboxyl groups. The presence of carboxyl groups attached to the silica surface enables the bioconjugates formation through covalent bonding of antibodies to the carboxyl-functionalized mesoporous silica.

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P3.21 Calcium-Modified Titanate Nanotubes for Photocatalytic Processes

Silviu Preda[1], Polona Umek[2], Crina Anastasescu[1], Valentin-Adrian Maraloiu[3], Veronica Brătan[1], Jeanina Pandele-Cușu[1], Ioan Balint[1]
1.“Ilie Murgulescu” Institute of Physical Chemistry, Romanian Academy, 202SplaiulIndependentei, 060021, Bucharest, Romania
2. Jožef Stefan Institute, Jamova cesta 39, SI-1000 Ljubljana, Slovenia
3. National Institute of Materials Physics, 405A Atomiştilor, PO Box MG 7, 077125 Măgurele, Romania

Sodium titanate nanotubes were prepared from commercial anatase TiO_2, which was homogenized in aqueous NaOH solution and then treated in a microwave reactor at temperature up to 135 ^oC for 180 min. Protonated titanate nanotubes were subsequently obtained by repeated washing with distilled water and 0.1 N HCl, followed by drying at 100 °C. Calcium-modified sample of the protonated nanotubes was carried out by hydrothermal treatment at 140 °C for 3 h. A second sample, consisting of CaTiO3 nanorods, was prepared by hydrothermal treatment of the protonated titanate nanotubes in $Ca(OH)_2$ solution at 180 °C for 48 h; CaO was also identified as a secondary product.
The photogeneration of reactive oxygen species (ROS), including hydroxyl radicals (•OH) and superoxide radical anions (O2•−), and the mineralization of organic compounds were investigated under simulated solar light irradiation. Water splitting was additionally performed under UV exposure. The morphological, structural, and physicochemical properties of the materials were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), UV–Vis spectroscopy, photoluminescence (PL) spectroscopy, and zeta potential measurements.

P3.22 Fine Structural Modulation Drives Circularly Polarized Luminescence in Helicoidal Zn(II) Coordination Polymers

Catalin Maxim[1,3], Cristiana Dabija[1], Victor Dobrilă[1], Cristian D. Ene[2]
1. Faculty of Chemistry, University of Bucharest, 4-12 Regina Elisabeta Blvd, 030018-Bucharest, Romania.
2. ”Ilie Murgulescu” Institute of Physical Chemistry, Romanian Academy, Coordination and Supramolecular Chemistry Laboratory, 202 SplaiulIndependentei, 060021 Bucharest, Romania.
3. “Costin D. Nenitescu” Institute of Organic and Supramolecular Chemistry of the Romanian Academy, 202B SplaiulIndependentei, 060023Bucharest, Romania.

Chirality plays a decisive, albeit low-profile role in various scientific disciplines, including chemistry, biology, and materials science. Tuning the chiroptical properties is achieved by altering the optical activity of the involved chiral molecules through external stimuli such as light, temperature, electric/magnetic fields, and chemical environment. This manipulation can lead to changes in the magnitude and/or direction of chiroptical responses and consequently offers new opportunities for controlling molecular chirality and designing functional materials with tunable optical properties. The most reliable strategy for introducing the chiral information into a metal ion-based network consists in employing an enantiomerically pure ligand. In this respect, the usage of natural amino acids is a straightforward and effective alternative. The study to be presented focuses on a set of tridentate salicylaldimine-type ligands containing different halogen substituents of the aromatic ring. As highlights, we mention: (i) the supramolecular architectures of simple organic chiral Schiff base, (ii) the Zn(II) helices assembled by exploiting these organic compounds as ligands, (iii) their optical properties (UV-Vis, PL, CD, and CPL spectra).

P3.23 Effect of the Concentration of Hyaluronic Acid on the Pharmacotehnical Properties of Carbopol-Based Hydrogels

*Izabela Dana Maria Stan[1], Emma Adriana Ozon[2], Adina Magdalena Musuc[1]**
1.“Ilie Murgulescu” Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021, Bucharest, Romania
2. Faculty of Pharmacy, “Carol Davila” University of Medicine and Pharmacy, 6 Traian Vuia St., 020956 Bucharest, Romania
Corresponding author: amusuc@icf.ro

Recently, hydrogels based on biocompatible polymers have attracted considerable interest in applications as topical systems for wound management due to their ability to provide a hydrated environment and to facilitate the incorporation and delivery of active pharmaceutical ingredients (API) [1,2]. In the present study, Carbopol-based hydrogel formulations containing different concentrations of hyaluronic acid (HA) were developed and comparatively evaluated as potential candidates for biomedical applications. High molecular weight hyaluronic acid, an anionic polymer, due to the increased size of the molecules, has the ability does not penetrate the deep layers of the skin, acting on the surface and having immediate benefits of hydration and protection [3]. The developed systems were further subjected to pharmacotechnical evaluation, including macroscopic appearance, homogeneity, pH, spreadability, and viscosity, to assess the influence of HA concentration on the performance and handling characteristics of the Carbopol-based hydrogels. The results demonstrated that the incorporation of HA modified the pharmacotechnical properties of the Carbopol-based systems depending on the concentration of hyaluronic acid. Changes in viscosity and spreadability were most relevant to establish the appropriate balance among the stability of the developed formulation, ease of application, and resistance in time on the skin. The obtained results allowed the identification of an optimal formulation with suitable characteristics for further development as topical hydrogel systems.

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P3.24 Smart Microbial Polysaccharide Hydrogels for SustainableDecontamination of Antibiotic-Contaminated Waters

*Ioana Cătălina Gîfu, Lucian-Gabriel Zamfir, Cristina Firincă, Iuliana Răut, Mariana Constantin, Andreea Luiza Mîrț, Mihaela Doni, Ana-Maria Gurban**
INCDCP- ICECHIM, Department of Biotechnology, 202 SplaiulIndependentei, 0600021,Bucharest, Romania
Corresponding author: ana-maria.gurban@icechim.ro

The continuous increase of antibiotic residues in water and food poses significant environmental and public health risks, highlighting the need for efficient and sustainable decontamination methods. Removing antibiotics from water is difficult to achieve with maximum efficiency, as they belong to different chemical classes and exhibit distinct physicochemical properties, such as polarity, solubility, electric charge, and the ability to interact with organic matter and mineral surfaces. In the aquatic environment, their concentration and persistence are influenced by complex processes, including adsorption, photolysis, chemical transformations, and biodegradation. One of the efficient methods to decontamination of polluted water is to use hybrid hydrogels [1,2]. This study presents the development of innovative hybrid materials that combine natural polysaccharides with inorganic clay fillers, demonstrating a high specific surface area and functional versatility for the simultaneous adsorption and biodegradation of pharmaceutical residues in polluted waters. The present study investigates the effect of clay content on the physicochemical properties of the new hydrogels, as well as their efficiency in removing antibiotics.
Physicochemical characterization showed that these innovative hydrogels exhibit adsorption capacities of 50 to 500 mg/g for tetracycline, depending on the crosslinking degree and functionalization, with removal efficiencies of 90% under optimal pH and dosage conditions. Adsorption kinetics follow a pseudo-second-order model, indicating chemisorption dominance. Hydrogels also demonstrate good regeneration, maintaining high efficiency over multiple cycles, supporting their sustainability for water treatment. These results confirm the potential of polysaccharide-clay hybrid hydrogels as sustainable and reusable materials for the effective decontamination of water contaminated with pharmaceutical residues, opening up promising prospects for large-scale applications in water treatment.

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P3.25 Nano-mechanical Assessment of Polyvinyl Alcohol Hydrogels Embedding Hafnia-Based Nanostructured Powders

Mihai Anastasescu, Daiana Mitrea, Hermine Stroescu, Madalina Nicolescu, Veronica Bratan, Radu Socoteanu, Crina Anastasescu, Maria Zaharescu, Ioan Balint*
"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021, Bucharest, Romania
Corresponding author: manastasescu@icf.ro

The development and optimization of advanced functional materials that can be integrated with clean energy sources, such as sunlight, are essential for current research with high applicability. This work presents the morphological and nano-mechanical characterization of PVA hydrogels processed as thin films, deposited on glass substrates, which incorporate hafnium oxide and silica powders. Characterization of these hydrogel films by nano-indentation is essential to accurately map their localized elastic behavior and evaluate their interfacial adhesion to the substrate, key factors that ensure their structural integrity and operational performance in different applications. This strategy extends the utility of the hafnium based oxides beyond the conventional dielectric role, to new photoactive functional platforms. Atomic Force Microscopy was used to obtain high-resolution micrographs of PVA hydrogels on glass substrates, formed by incorporating hafnia-based powders, as well as to analyze the nanoscale mechanical behavior of these hydrogels through force-distance spectroscopy experiments. Evaluating Hf-based hydrogel films through force-distance spectroscopy using Hertz, JKR, and Sneddon contact models revealed strong tip-matrix interactions and adhesion-dominated energy dissipation, underscoring the need for viscoelastic analysis. The resulting mechanical softening and energy loss confirm that residual moisture plasticizes the PVA matrix, shifting its elastic modulus from

the GPa to the MPa scale while boosting polymer chain mobility and hydrogen bonding to promote high adhesion energy.

P3.26 Ni and Ag Doped TiO_2 Nanopowders Prepared by the Sol-Gel Method for Stable Water-Based Nanofluids

Luminița Predoană[1], Jeanina Pandele-Cusu[1], Irina Atkinson[1], Oana Cătălina Mocioiu[1], Zalán István Várady[2], Bence Kun[2], Emese Mesterné Kurovics[3], Gábor Karacs[4], Benjámin Sándor Gyarmati[5], Diána Balogh[6], Marcell Bohus[2], Imre M. Szilágyi[4], Maria Zaharescu[1]

1. "Ilie Murgulescu" Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania
2. Department of Inorganic and Analytical Chemistry Budapest University of Technology and Economics, Budapest, Hungary
3. Institute of Energy, Ceramics and Polymer Technology, University of Miskolc, Miskolc, Hungary
4. Institute of Physical Metallurgy, Metal Forming and Nanotechnology, University of Miskolc, HU-3515 Miskolc-Egyetemvaros, Miskolc, Hungary
5. Department of Physical Chemistry and Materials Science, Faculty of Chemical Technology and Biotechnology, Budapest University of Technology and Economics, Budapest, Hungary
6. Department of Organic Chemistry and Technology, Faculty of Chemical Technology and Biotechnology, Budapest University of Technology and Economics, Budapest, Hungary

Pristine and Ni- or Ag-doped TiO_2 nanopowders were prepared by the sol-gel method and investigated as functional materials for the obtained water-based nanofluids. TiO_2 powders containing 1, 2, and 4 mol% of Ni or Ag were prepared, thermally treated, and subsequently dispersed in water. The study focused on establishing the relationship between the synthesis conditions, structural characteristics of the nanopowders, and the colloidal stability of the resulting nanofluids. Thermal analysis was employed to determine the appropriate heat-treatment conditions, indicating that 600 °C was suitable for the removal of organic species and the formation of crystalline phases. The synthesized materials were characterized by X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR) to assess their crystalline structure, average crystallite size, and chemical bonding. The particle density was determined using a pycnometric method. The stability of the TiO_2-based aqueous nanofluids was evaluated by zeta-potential measurements. The undoped and doped particles exhibited acceptable aggregative stability in water without additional stabilizers, the incorporation of 0.5 mass% sodium carboxymethyl cellulose (NaCMC) significantly enhanced the dispersion stability, resulting in zeta-potential values of approximately −60 mV. The results demonstrate that the combination of sol-gel synthesis, controlled doping, and polymer-assisted stabilization provides a suitable strategy for obtaining stable TiO_2-based nanofluids.

P3.27 Advanced characterization of crystalline oxide materials withimproved electrical and photocatalytic properties

Oana Cătălina Mocioiu[1], Irina Atkinson[1], Veronica Brătan[1], Ana-MariaMocioiu[2], Jeanina Cuşu-Pandele[1], Cristina Maria Vlăduț[1], Elena MirabelaSoare[1], Sorana Elena Lazăr[1], Cristian Hornoiu[1]*

1. "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 SplaiulIndependentei, 060021, Bucharest, Romania
2.National Research & Development Institute for Non-ferrous and Rare Metals- IMNR, 102 Biruinţei Boulevard, Pantelimon, 077145 Ilfov, Romania
Corresponding author: omocioiu@icf.ro

In this work we studied the electrical and photocatalytic properties of crystalline oxide materials based on ZnO obtained by solid state reaction at 1173K. Structure of the studied materials was determined by X-ray Diffraction with JCPDS cards and Fourier Transform Infrared Spectroscopy. The morphology of the materials observed by Scanning Electron Microscopy showed particles in the 400-600 nm range. Differential thermal analysis (DTA) and thermal gravimetry (TG) was used to establish their thermal behaviour. All TG curves show an increase in mass simultaneously with effects in DTA probably due to oxygen adsorption in the materials during heating. Electrochemical Impedance Spectra (EIS) recorded led to the conclusion that temperature introduces oxygen defects in materials that will greatly improve the separation capacity of generated carriers, phase formation and electrical properties. Nyquist plots of the materials at different temperatures 673K, 873K and 1173K show the improve of electrical properties with increase of temperature. The presence of high ZnO content in the composition of the studied materials increase the BB decomposition efficiency.

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P3.28 Pencil Graphite – a Versatile Electrode Material for Rapid Fluoroquinolone Screening

Mihaela Bănică[1], Daniela Partene [1,2], Iulia-Gabriela David[1,3]

1. Department of Analytical Chemistry and Physical Chemistry, Faculty of Chemistry, University of Bucharest, Panduri Av. 90-92, District 5, 050663 Bucharest, Romania

2. Doctoral School of Chemistry, University of Bucharest, 4-12 Regina Elisabeta Boulevard, 030018 Bucharest, Romania
3. Research Centre for Applied Analytical Chemistry, Faculty of Chemistry, University of Bucharest, Panduri Av. 90-92, District 5, 050663 Bucharest, Romania

Pencil graphite electrodes (PGEs) are increasingly used in electroanalytical applications because they are inexpensive, readily available, easy to handle, and suitable for disposable use. Pencil leads are composite materials containing graphite, clay, and a binder, and their properties depend on the graphite-to-clay ratio. An important advantage of these electrodes is the possibility of renewing the working surface simply by replacing the pencil lead, without the polishing steps usually required for conventional solid electrodes. Their use also allows the electrode preparation procedure to remain simple, with low reagent consumption and reduced preparation time. For carbon-based electrodes, electrochemical activation is a convenient way to improve the surface properties without requiring a complex modification procedure.

In this work, an HB-type pencil graphite electrode was electroactivatedpotentiostatically in phosphate-buffered solution (PBS) by applying 2.00 V for 60 s, and the resulting electrode was denoted as HB_PGE*. The electroactivated electrode was then tested for the voltammetric determination of norfloxacin (NOR). NOR is a fluoroquinolone antibiotic widely used in both human and veterinary medicine. Its presence has been reported in municipal and hospital wastewater, making its monitoring relevant from both analytical and environmental perspectives. The development of simple methods for its detection is therefore of interest, particularly for rapid screening and quantitative analysis.

The electrochemical behavior of NOR was studied under different experimental conditions. The oxidation response was influenced by the pH of the supporting electrolyte, with the highest anodic peak current obtained in PBS at pH 6.50. Studies performed at different scan rates indicated that both adsorption and diffusion contribute to the electrochemical response. Quantitative determination of NOR was carried out by differential pulse voltammetry (DPV) and adsorptive stripping differential pulse voltammetry (AdSDPV). Good linear responses were obtained with both techniques, with sensitivities of 0.364 $A \times L \times mol^{-1}$ for DPV and 2.3341 $A \times L \times mol^{-1}$ for AdSDPV. The higher sensitivity observed for AdSDPV is related to the accumulation of NOR at the electrode surface before the voltammetric measurement. With an accumulation time of 30 s, a limit of quantification of 7.77×10^{-7} M was obtained. The HB_PGE* also showed good repeatability and was successfully applied to the determination of NOR in commercial pharmaceutical tablets.

Overall, the study shows that a commercially available pencil graphite lead, combined with a short and simple electrochemical activation step, can provide a suitable electrode for NOR determination. The low cost, disposable character, minimal reagent consumption, and short preparation time make the HB_PGE* a promising material for rapid fluoroquinolone screening and pharmaceutical quality control.