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ABSTRACT BOOK

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PLENARY LECTURES

PLENARY LECTURES

Fishing and fish trade at the lower Danube. Historical perspectives and lessons for today

C. Ardeleanu

The Lower Danube University of Galati

This presentation is a historical overview of fishing and fish trade at the Lower Danube from the ancient times until the 20th century. Fishing has always been an important occupation of the local communities, and historical sources refer to the abundance and cheapness of fish in the ports of Moldavia and Wallachia. Sturgeons and caviar represented part of the common trading products provided by merchants from this area, and they were famous on many Mediterranean and Western European markets. However, overfishing became a reality in the 19th century, and the first regulations for protecting fish populations became necessary. All in all, such a historical approach is essential when trying to understand contemporary problems of endangered fish species.

Functionalized graphene for environmental and biomedical applications

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Recent developments in materials science and nanotechnology have propelled the development of a plethora of materials with unique chemical and physical properties for various applications. Particularly, graphitic nanomaterials such as carbon nanotubes, fullerenes and, more recently, graphene oxide (GO), and reduced graphene oxide (rGO) have gained a great deal of interest for their potential applications in various aspects of science and technology.

Graphene, the name specified to a one atom-thick two-dimensional (2D) single layer of sp^2 hybridized carbon atoms arranged in a honeycomb lattice with large surface area, exceptional thermal, mechanical, optical and structural properties. This wonder material and its derivatives have generated great attention in different areas of research for their potential applications in several fields such as nano-electronics, organic catalysis, environmental remediation, drug delivery, etc.

Due to their low cost of production, large specific surface area and abundant surface chemistry, GO and rGO have shown great promise in the development of novel composites. These hybrid nanomaterials offer unusual combinations of electrical, thermal, mechanical, catalytic, optical and magnetic performances that are difficult to attain separately from the individual components.

In this presentation, I will focus on the different strategies for the preparation of rGO hybrid materials and the various applications of these nanohybrids in biomedicine, biosensing, energy storage, and environmental remediation.

Advanced concepts of photovoltaics based on III-V compounds and hybrid perovskites

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With 25.6% conversion efficiency, solar cells based on the c-Si generation reach their limits. However, the third generation solar cells, such as multijunction solar cells and hot-carrier solar cells (HCSCs), allow to overcome the intrinsic limit of a single junction. Firstly, we show the first stage developments of a GaAsPN/Si tandem cell on Si, which benefit from the low cost and technological maturity of Si cells. The GaAsPN dilute-nitride compound, grown by MBE, is quasi lattice-matched with Si, and displays the required the required 1.7 eV pseudo-bandgap. Secondly, HCSCs aim to reduce the thermalization process which is a major loss in a classical PV cells. This can be done by the reduction of the electron-phonons interactions in quantum wells (QWs) structures. Therefore, we have investigated a InGaAsP multi-QWs heterostructure epitaxially grown on a InP(001) substrate and demonstrate its potential to work as a hot carrier cell absorber. Finally, some outstanding properties of the hybrid organic perovskites, a very new technology which has quickly reached conversion efficiency larger than 20%, will be presented, along with results from a collaboration between FOTON laboratory, Los Alamos National Laboratory, Rutgers University New Jersey, Purdue university, Brookhaven National Laboratory and Chemical Sciences Institute of Rennes.

Electrochemical application of Boron-doped diamond electrodes

Yasuaki Einaga

Department of Chemistry, Keio University, Japan

Boron-doped diamond (BDD) electrodes are very attractive material, because of their wide potential window, low background current, chemical inertness, and mechanical durability[1]. In these years, we have reported several examples for electrochemical sensor applications[2]. Here, we report some recent examples of electrochemical sensor application of BDD such as ozone [3], pH [4], in vivo detection of neurotransmitter in monkey brain [5], and in vivo detection of glutathione for assessment of cancerous tumors [6] using BDD microelectrodes. Furthermore, other applications such as organic synthesis [7], ozone generation, and CO₂ reduction [8] are also shown. Furthermore, in order to understand the fundamental properties, the effect of sp²-bonded carbon impurities on the electrochemical properties of BDD were investigated in moderately ([B] < 10²⁰ cm⁻³) and heavily ([B] > 10²¹ cm⁻³) boron doping levels for the applications.[9]

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XRD and luminescence properties of nanocrystalline hexagonal Boron Nitride powders

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Nanocrystalline hexagonal boron nitride powders (h-BN) were synthesized from urea and boric acid followed by pyrolysis and subsequent heat treatment in nitrogen atmosphere. Materials have been analyzed by means of X-ray diffraction, Photoluminescence and Field emission electron microscopy methods. Obtained results show that starting h-BN powder, synthesized at 750 °C, is composed of ~11 layer crystallites with average crystallite thickness and crystallite lateral size of 3.94 and 10.4 nm, respectively. A broad emission and intense luminescence intensity were observed due to the large atomic disorder. Higher annealing temperature increases crystallite size and turbostratic h-BN transforms to well crystallized h-BN at 1500 °C. This simple and effective method can be used to prepare boron nitride in large scale.

Investigation of solid phase crystallization and of optical properties of HfO₂ thin films

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During the recent years, there has been a growing interest in the study of the physical properties of metal oxides and hafnium dioxide (HfO₂) in particular due to their important technological applications CMOS and RF microelectronics technologies, the manufacture of interference coatings in the UV spectral range down to 250nm and have been previously used for gas and magnetic field sensors. In this talk we will discuss the microstructural and optical properties of amorphous HfO₂ films obtained by Plasma Ion Assisted Deposition and Atomic Layer Deposition. The optical properties were studied by variable angle spectroscopic ellipsometry in the visible spectral range, while the structural properties were analyzed with grazing-incidence x-ray diffraction and x-ray reflectometry, Raman and FTIR spectroscopies. We will discuss the solid phase crystallization of amorphous HfO₂ thin films following thermal annealing.

The experimental results show a clear correlation between the optical properties and the variations of the structural properties due to the annealing. Thus, the as-deposited layers show a poor crystalline state, with a low refractive index and energy band-gap. As the annealing temperature was augmented, the degree of crystallinity was increased, as well as the refractive index and the band-gap. Moreover, the annealing also induced a reduction of the layer thickness and a slight increase of the surface roughness. The crystalline grains consist of cubic and monoclinic phases already classified in literature but this work provides the first evidence of amorphous-cubic phase transition at a temperature as low as 500 degrees C.

Nanomagnetism: Superparamagnetism in Iron - doped CeO_{2-y} nanocrystals

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Magnetic properties of materials fundamentally change when the particle sizes are reduced [1]. Below a critical size (D_C), which typically lies below 100 nm, normal microscopic multidomain ferromagnetic (FM) structure is energetically unfavorable, and the particles are in single domain state. In this state, the mechanism of magnetization reversal can only occur via the rotation of the magnetization vector from one easy magnetic direction to another over the magnetic anisotropy barrier [2]. As particle size decreases within the single domain range, another critical threshold (D_{SP}) is reached, at which remanence and coercivity go to zero and the particles are in the superparamagnetic (SP) state. Such a system has no hysteresis and magnetization curves at different temperatures superimpose onto a universal curve of M/M_S vs H/T (Langevin's curve).

We have measured the magnetization of undoped and Fe^{2+/3+} doped CeO_{2-y} nanocrystals at various temperatures and magnetic fields [3]. In the case of Fe-doped samples, the superparamagnetic behavior of this system is revealed by nearly zero coercive field, an appearance of the blocking temperature below 20 K, as well as the $M(H)$ dependence, which is well fitted by weighted Langevin function which takes into account particle magnetic moment distribution [3].

We have also measured Raman scattering spectra of these nanocrystalline samples. Raman mode exhibits softening and broadening by changing the valence state of Fe dopant, as a consequence of the electron-molecular vibration coupling. The electron-molecular vibration (phonon) coupling constants λ and density of electron states at the Fermi level per spin and molecule $N(0)=22$ (eV)⁻¹ were determined. The Stoner condition $N(0)I > 1$ is multiple fulfilled in the case of nano CeO_{2-y} favoring the band ferromagnetism approach [4].

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PLENARY LECTURES

History of sol-gel preparation of some functional materials

Sumio Sakka

Professor Emeritus of Kyoto University

Sol-gel processing for fabricating materials is characterized by starting with a solution. Compounds contained in the solution as source of materials undergo hydrolysis and condensation near room temperature, forming gel products. Heating of gels to several hundred degrees or higher temperatures produces dense oxide glasses and ceramics as final products. Significant sol-gel works started around 1970 with the purpose of preparing homogeneous glasses and ceramics. Invention of sol-gel preparation of organic-inorganic hybrid materials in 1984 broadened the area of sol-gel derived materials, and around 1995 this resulted in attracting people working in all the material-related technology areas. Since then, the sol-gel method has been regarded as one of the most powerful means for fabricating functional materials including photonic, electronic, chemical, mechanical and biomedical materials. Furthermore, sol-gel method itself has been experienced much progress in the process of the application to fabrication of materials. In sol-gel processing we can provide the resultant materials with varying microstructures, such as amorphous, polycrystalline and single-crystalline ones. The grain size of polycrystalline ceramics can be varied. Also, nature of precipitated crystals and precise modification of chemical composition are possible in the sol-gel processing. These features of the sol-gel method will be explained through the historical development of sol-gel derived ferroelectric materials and TiO₂-based solar cells.

Structural speciation and structure-property correlations in binary-ternary coordination polymers Pb(II) with di-/tricarboxylic acids

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Metal-organic hybrid functional materials attract considerable interest toward potential applications, emanating from innate relationships between structural and spectroscopic properties, further supported by extensive chemical reactivity. In order to delineate such complex structure-property relationships, leading to the development of Pb(II)-containing metal-organic coordination polymer materials supporting metal-organic technology, a systematic investigation of binary-ternary Pb(II)-di-/tricarboxylic acid systems involving aromatic N,N'-chelators bipyridine(bpy)/phenanthroline(phen) has taken place through pH-specific hydrothermal synthetic efforts. The organic acid ligands chosen were a) aliphatic $\text{HOOC}(\text{CH}_2)_n\text{RCOOH}$ acids, with variable spacer carbon chains, and b) aromatic carboxylic acids of variable yet distinctly modifiable structural motifs. The perused chemical reactivity afforded new crystalline metal-organic coordination polymeric and non-polymeric materials characterized by X-ray crystallography. Further detailed physicochemical characterization (elemental analysis, FT-IR, ^{13}C -, ^{207}Pb -CPMAS NMR, TGA, luminescence) reveals architecture, lattice dimensionality (2D-3D) and luminescence property correlations, thereby identifying distinct contributions of structural and electronic factors interweaving into the design of new functional materials linked to catalytic and optoelectronic applications.

PLENARY LECTURES

Engineered, tailor-made polymers for bio-related applications

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Last decades have witnessed an increased interest in the rational design of complex polymeric structures through new and well-controlled synthetic approaches. One of the main targets of this interest consists in the development of tailored polymer materials, engineered to exert distinct biological functions, implying multifunctionality as well as appropriate three-dimensional architectures.

Macromolecular structures including micelles, polymersomes, nano-/microparticles (-capsules/-spheres), dendrimers, nanogels, hydrogels, interpenetrated polymer networks have been developed and tested as potential systems of interest for bio-related applications. To gain clinical importance, such materials must respond to severe demands, often implying a combination of natural and synthetic polymers or composite materials (inorganic/organic, biocomposites), while the targeted application site or cargo may require specific material category (biodegradable, bioresorbable), dimension scale (micro/nano size) and topographic characteristics.

The presentation summarizes the history and challenges in polymers/materials addressing bio-related applications, pointing on polymers as a powerful solution to specific challenges and focusing on the newest strategies to improve systems effectiveness and responsiveness (design keys, preparative approaches). Controlled drug delivery and its application, gene therapy and tissue engineering will be presented as important polymer contributions to bio-related areas. Expected future directions will be underlined.

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PLENARY LECTURES

Certainty and uncertainty of thermodynamic data

M. Stan

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Thermodynamic data is among the most complex in modern science and technology and presents large uncertainty at multiple length and time scales. Given the disparity of data sources, interaction complexity, and the lack of rigorous thermodynamic correlations, there is a recent focus on synergistic investigations combining experimental measurements and computational results. A distinguishing feature of thermodynamic data is that uncertainty sources go beyond experimental data and mathematical models and include provenance features such as types of biases of given instruments, calculations, and research groups; the later are rarely included in uncertainty evaluations. We discuss the role of Bayesian analysis in learning and understanding different types of thermodynamic data and its provenance, as well as the incompleteness of existing data sets. The methodology allows for consistent inclusion of heterogeneous input information such as experimental and computational enthalpy, entropy, free energy, reaction rates, and phase diagram features that are related via thermodynamic relationships. This approach accounts for the errors associated with reported data and how reliable the researcher believes the models to be. We also discuss the partnership between humans and machines in analyzing and understanding thermodynamic data, including computational tools that take advantage of high performance computing capabilities to learn from existing data, evaluate uncertainty while maintaining thermodynamic self-consistency, and propose the most informative new experiments and computations.

Dipole ordering and its interplay with spin-orbit coupling in perovskite halide solar cells

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Ferroelectricity is a potentially crucial issue in halide perovskites, breakthrough materials in photovoltaic research. Using density functional theory simulations and symmetry analysis, we show that the lead-free perovskite iodide (FA)SnI₃, containing the planar formamidinium cation FA, (NH₂CHNH₂)⁺, is ferroelectric. In fact, the perpendicular arrangement of FA planes, leading to a 'weak' polarization, is energetically more stable than parallel arrangements of FA planes, being either antiferroelectric or 'strong' ferroelectric. Moreover, we show that the 'weak' and 'strong' ferroelectric states with the polar axis along different crystallographic directions are energetically competing. Therefore, at least at low temperature, an electric field could stabilize different states with the polarization rotated by $\pi/4$, resulting in a highly tunable ferroelectricity appealing for multistate logic. Intriguingly, the relatively strong spin-orbit coupling in noncentrosymmetric (FA)SnI₃ gives rise to a co-existence of Rashba and Dresselhaus effects and to a spin texture that can be induced, tuned and switched by an electric field controlling the ferroelectric state.

A. Stroppa et al. *Nature Communications* **2015**, *5*, 5900.

PLENARY LECTURES

Danube sturgeons - Current status and conservation measures

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Only five out of six former existing species of sturgeons still survive in the Danube River but only three long-migratory and one resident freshwater species (sterlet) continue to spawn in the Lower Danube River. Following a period of 10 years (1990 - 2000) of unregulated and uncontrolled fishing, despite regulations adopted in year 2001 and five years of implementation of regulations adopted by the Convention on International Trade in Endangered Species of Wild Fauna and Flora (CITES), stocks of sturgeon populations were declining dramatically. Romanian authorities for environment and agriculture adopted in May 2006 a ten year moratorium on commercial catches of sturgeons and started to implement on annual basis (2006 - 2019) supportive stocking of the river using young sturgeons obtained by controlled propagation of wild brood stock captured in the river. In year 2010, due to financial shortages and the impossibility to conduct comprehensive evaluation of the stocking procedures and results, the supportive stocking programme was discontinued. The Lower Danube University of Galatz started in year 2013 a large scale in situ pilot project, funded by the Romanian Fishery Operational Programme (FOP), to evaluate the survival and distribution of young sturgeons stocked experimentally in different locations of the Lower Danube River. The main results of the evaluation were that young sturgeons stocked in the river adapt well to feed and grow well in the wild environment. Continuation of the commercial catch moratorium for the next 5 years (2016 - 2020) was adopted by a regional meeting of CITES and fishery authorities held in Bucharest in November 2015.

SECTION 1

Theoretical chemistry. Molecular spectroscopy.

KEYNOTES

Complexation of TEMPO derivatives with cyclodextrins assessed by EPR spectroscopy, circular dichroism and DFT calculations

I. Matei, M. V. Neacsu, S. Mocanu and G. Ionita

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We explore here the interaction of the spin probe 2,2,6,6-tetramethylpiperidine 1-oxyl (TEMPO) and two of its derivatives, 4-amino- and 4-carboxy-TEMPO, with α -, β -, 2-hydroxypropyl- β - and γ -cyclodextrins, in neutral, acidic and basic conditions. By means of electron paramagnetic resonance (EPR) spectroscopy, we show that the affinity of the spin probe for the cyclodextrin cavity is influenced by the type and protonation state of the functional group attached to the TEMPO moiety. The species prone to complexation are identified, and the association constants and stoichiometries of the interactions are determined. The EPR data at room temperature and at low temperature in frozen solutions are complemented by information obtained by circular dichroism. Neutral 4-amino-TEMPO and 4-carboxy-TEMPO give induced circular dichroism signals upon interaction with cyclodextrins. The spectral features of these dichroic signals (band signs and positions) and the EPR parameters of the spin probes are further correlated to the results of molecular docking and density functional theory (DFT) calculations, allowing us to elucidate the geometry of the inclusion complexes.

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Complexation of β -cyclodextrin with dual molecular probes bearing florescent and paramagnetic moieties linked by short polyether chains

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Molecular probes can yield valuable information at nanoscale level of various systems that are macroscopically homogeneous. Dual molecular probes have the advantage of using two different methods to provide information on the microenvironment of the probe and interactions with other species. A series of dual molecular probes (denoted PyTEGn) bearing fluorescent and paramagnetic moieties linked by flexible short polyether chains ($n = 1-6$) have been obtained.

EPR and fluorescence methods were employed to investigate: *i*) the quenching effect exercised by nitroxide moiety on the pyrene fluorescence as a function of linker properties and *ii*) the interaction of these molecular probes with cyclodextrins, in solution and in polymeric gels.

Rotational correlational time (τ) and fluorescence quantum yields of PyTEGn (Φ) vary non-uniform with the length of the oligo-ethylene oxide chain. This behaviour is due to linker flexibility. The fluorescence quenching induced by the nitroxide moiety depends on the chain length and conformation of the linker.

The analyses of EPR and fluorescence spectra of PyTEGn in the presence and in the absence of cyclodextrins provide information on the stoichiometry and assembly of the host-guest complexes.

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SECTION 1

Theoretical chemistry. Molecular spectroscopy.

POSTERS

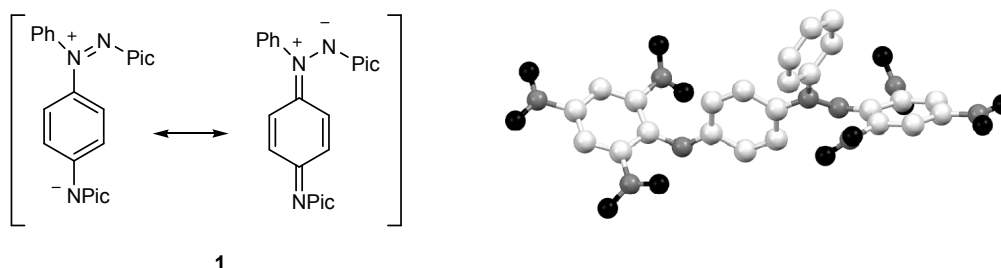
Properties of the blue dye 1-picryl-2-phenyl-2-(4-picrylamidephenyl)-diazonium betaine

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We investigated the physico-chemical properties of the title deep blue coloured betainic dye (**1**) in the solid state and in solution. Due to a single crystal X-ray analysis we could correlate the observed bulk properties such as magnetism, visible absorption spectra, and the redox behaviour, to the peculiar molecular electronic structure, best represented by two formulas below, where Pic (picryl) stands for the 2,4,6-trinitrophenyl group.



Heterotopic luminescent sensors to alkali metals in aqueous media

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Series of new crown-substituted pyrroles and crowned porphyrins were tested as supramolecular sensors to sodium and potassium cations. We found that water-soluble magnesium(II) and aluminum(III) crowned porphyrins can bind effectively potassium cations in aqueous media by forming of sandwich-type supramolecules. Binding of potassium cations by the crowned porphyrin molecule leads to strong changes of color (from pink to green). Changes of UV-Vis and luminescence spectra were analyzed for the process and the sensitivity of the molecule-receptor to potassium cations was estimated.

One more interesting phenomenon was found for aluminum(III) crowned porphyrin. This compound manifests thermochromism in toluene solution. We analyzed changes of UV-Vis, luminescence spectra, light scattering data and proposed the mechanism of the process – formation of coordination polymer in toluene solution when cooled.

This work was supported by a grant of the Russian Academy of Science.

Designing and programming an artificial neural network model for the modeling/discrimination of amphetamines

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The goal of this paper was to develop an expert system capable of identifying the potential biological activity of new substances having a molecular structure similar to illicit amphetamines. To this purpose, we have designed fourteen artificial neural networks using Neural Network Toolbox, MATLAB 7.0.0, which have been trained to classify amphetamines according to their toxicological activity and to distinguish them from nonamphetamines based on their molecular descriptors, *i.e.* constitutional descriptors, functional group counts, atom-centred fragments, topological descriptors, walk and path counts, connectivity indices, information indices, Burden eigenvalues, edge adjacency indices, geometrical descriptors, RDF, WHIM, GETAWAY and 3D-MoRSE descriptors. Such a system is essential for testing new molecular structures for epidemiological, clinical, and forensic purposes. The efficiency of each network to identify the class identity of an unknown sample was evaluated by calculating several figures of merit. The relevance of each type of molecular descriptors in the modeling/discrimination of amphetamines is discussed.

Antioxidant property of some arylthio derivatives and their reaction with the stable free radical 2,2-diphenyl-1-picrylhydrazyl, DPPH

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The reactions of the stable free radical 2,2-diphenyl-1-picrylhydrazyl **DPPH (1)** with 2-mercaptobenzoxazole **2** and 2-mercaptobenzothiazole **3** have been investigated by UV-Vis spectroscopy and TLC. The antioxidant property of arylthio derivatives **2** and **3** has been calculated from UV-Vis data. The reaction products were isolated by TLC and characterized through physico-chemical methods: ¹H-NMR and ¹³C-NMR, IR, UV-Vis and ESR. The results of these analysis suggest the complexity of reaction mechanism leading to a series of new compounds.

Thermal degradation pathways of selected brominated flame retardants from first principles

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Chromatographic analyses of polybrominated diphenyl ethers (PBDEs) use temperatures above 300°C for their elution. Therefore, their thermal degradation occur influencing quantification accuracy from matrices related to human exposure to such compounds. Establishing the principal PBDEs degradation products to monitor for controlling chromatographic analysis is highly needed for improving methods accuracy.

Throughout this study, pathways to thermal decomposition of decabrominated diphenyl ether (BDE 209) were investigated by thermochemical computations at the density functional theory (DFT) level. Within DFT, a wide range of approximate density functionals/basis set combinations were first benchmarked against available experimental data in reproducing (aromatic) C-O and C-Br bond dissociation energies (DEs). Among the functionals considered, we find that M06 global meta-hybrid at either cc-pVnZ or aug-cc-pVnZ (n = D,T) perform the best in reproducing the two bond DEs with comparable yet <2 kcal/mol deviations from a set of consistent experimental references. Preliminary results on BDE 209 foresee a 10 kcal/mol lowering of the C-O DE w.r.t the un-brominated compound, whereas the C-Br DEs are predicted to differ (ortho > meta > para) within 1-2 kcal/mol.

Aknowledgements: This work was supported by a grant of CNCS-UEFISCDI, project number PN-II-RU-TE-2014-4-1010.

Improved chemometric evaluation of the chromatographic columns with respect to the separation of chemical classes

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A novel multivariate visualization approach, for the evaluation and comparison of the chromatographic systems is proposed, in order to connect the similarity/dissimilarity information, given by principal component analysis, to the selectivity of the sorbent material (*e.g* the separation factor). Algebraic conditions were obtained for the separation of chemical classes, in terms of the first two principal components derived from the solvation coefficients of a large set of chromatographic stationary phases. The points corresponding to the stationary phases and the condition for a certain separation between the structural features could be embedded into planar representations, by using the same coordinates system. The relative position of these two elements should account for the effective pair resolution on a given column, thus allowing a fast visual evaluation of the stationary phases with respect to a certain analytical purpose. These aspects were exemplified on several delicate separation questions, regarding chemical classes with resembling polarities.

The effect of non-gelator species on supramolecular assembly of low molecular weight gelator – the case of 12-hydroxystearic acid/ 16-hexadecanoic acid

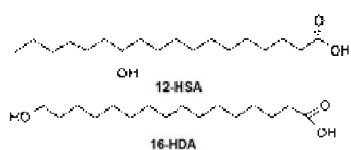
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An increasing number of organic compounds with low molecular weight (LMW) are found to be capable to unidirectional self-assembling into fibrous aggregates leading to a tridimensional network which can entrap solvents inside the interstices. These compounds are referred to as low molecular weight gelators (LMWGs) and often have chiral properties.

A classic example of LMWGs that induce gelation in a variety of organic solvents (toluene, benzyl benzoate, benzene, cyclohexane, *etc.*) is represented by 12-hydroxystearic acid (12-HSA). In



this study, we investigated the effect of a non-gelator, 16-hexadecanoic acid (16-HDA), on the properties of gels resulted by self-assembly of 12-HSA in benzyl benzoate. The physicochemical tools involved in this study were rheology, micro-DSC and IR spectroscopy measurements. Rheological data reveal that the presence of 16-HDA leads to the weakening of the gel network. Transition from sol-to-gel is an exothermic process and gelation temperatures shift to lower values in the presence of 16-HDA. IR spectra indicate that vibrations corresponding to CH₂ groups are sensitive to the sol-to-gel transition. All experimental data demonstrate that the presence of non-gelator molecule (16-HDA) inhibits the gelation process.

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Co(II) and Ni(II) complexes with ligands having antibacterial activity

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Both enrofloxacin and hydroxiquinoline have antibacterial activity. The use of these ligands together with phenantroline, in various molar ratios, to obtain complexes with Co(II) and Ni(II), is a promising route for synthesizing new compounds with pharmaceutical properties. The bacterial activity of these new metal complexes against various bacterial strains was determined by specific tests.

The geometries of all the possible complexes which can be formed in different solvents were evaluated by quantum chemistry calculations. There were taken into consideration the planar and tetrahedral complexes formed with two identical or different ligands, as well as the octahedral complexes formed with all the studied ligands in various molar ratios. There were performed Hartree-Fock calculations using GAMESS software package. The solvent effect was taken into account using the continuum environment approximation of Onsager. In the optimizing geometry processes there were used better and better wave functions starting with STO 3G and finishing with valence triple zeta (TZV). In this way the most probable geometries of the synthesized complexes were established.

Computed molecular descriptors and QSAR properties prediction on N-(p-iodophenyl)-N'-(2-tenoil)-thiourea

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A computational study using Spartan¹⁴ software Wavefunction, Inc. Irvine CA USA was conducted on the 3D optimized structure as CPK model (ball-and-spoke) of the compound N-(p-iodophenyl)-N'-(2-tenoil)-thiourea, presenting potential antimicrobial activity¹. Conformational analysis was performed to find the more stable conformer, presenting the energy minima and optimized geometry. Structure dependent indicators: the octanol-water partition coefficient (logP), the number of hydrogen bond donors (HBDs) and acceptors (HBAs), polarizability, HOMO-LUMO gap, dipole moment, number of tautomers and conformers. In addition, properties obtained from a space-filling model that are particularly valuable in QSAR type analyses have been calculated: area, volume, polar surface area (PSA), ovality. Their values resulted using the Hartree-Fock method², 6-31G* basis set³, in vacuum and in water for equilibrium geometry at ground state of the studied compound. Data have been interpreted in terms of electronic effects, molecular deformability, steric factors and reactivity, aiming to initiate further docking studies.

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1) C. D. Badiceanu, *et al.*, Rom. Biotech. Lett. 15 (2010) 5545. 2) W. J. Hehre, *et al.*, *Ab Initio Molecular Orbital Theory*, Wiley, New York, 1985. 3) R. Ditchfield, *et al.*, J. Chem. Phys. 54 (1971) 724.

Conformational studies of some new thiourea derivatives

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There were synthesized five new thiourea derivatives, which were characterized by different structural methods. Their antimicrobial actions were proven by specific appropriate methods.

The conformations of all thiourea derivatives were studied by quantum chemistry methods. For each compound 32 different conformers were generated taking into account its flexible structure. The geometry of each conformer was firstly optimized by the Hartree-Fock method using increasingly complex wavefunctions. Because many conformers have crooked geometries, the final geometry of each compound has been established by the DFT method performing B97D/6-31G(d,p) calculations, taking into account the London dispersion corrections.

The conformer ground states for each thiourea derivative cover a range of 25–30 kcal/mol, in all cases the conformer with lowest energy being a lying quasi-linear structure. In all cases, the geometry change from one conformer to another needs a large activation energy. Due to this fact, any conformer is stable enough.

We noted that in the cases of all five thiourea derivatives, the conformers with the lowest energy form inclusion complexes with both α - and β -cyclodextrins. Preliminary studies showed that the crooked structures also form inclusion complexes. In our opinion this is an expected result, taking into account that both the thiourea derivatives and cyclodextrin cavity have a hydrophobic character.

SECTION 2

Chemical kinetics and thermodynamics

KEYNOTES

Phase transitions of a parchment: A calorimetric and kinetic analysis

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To further understand the thermal stability of a parchment manufactured from deer skin, DSC measurements carried out on this biomaterial at several heating rates were used for kinetic analysis of the endothermic processes of denaturation in water excess and of the phase transition in dry state. The last process could be attributed to melting of crystalline (rigid) zone of parchment or the denaturation consisting in the evaporation of residual strongly bond water and continued conformational changes of super-helix of collagen that is the main component of parchment.

The kinetic analyses of non-isothermal DSC data were performed by Kissinger, isoconversional and “multivariate non-linear regression” (Multivar-NLR) methods. The application of isoconversional methods (Friedman, and Ozawa-Flynn-Wall methods) put in evidence that for both investigated processes the apparent activation energy decreases with the degree of phase transition. This suggests that the investigated processes exhibit Lumry-Eyring mechanism, consisting in a reversible process followed by an irreversible one. The application of Multivar-NLR method confirms this suggestion. According to the results obtaining by kinetic analysis, the process occurring in dry state seems to be a denaturation than a melting of crystalline (rigid) zone of parchment.

Acknowledgements

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Kinetic models for oxidation of nuclear graphite by moisture in Helium coolant

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High purity, near-isotropic graphite is used as structural element and neutron moderator in high temperature gas-cooled reactors (HTGRs). Traces of moisture might be present in the high purity helium coolant and will inevitably cause extremely slow and continuous oxidation of graphite. This chronic process may cause structural damage over the life time of nuclear power plants. For the safe design and operation of HTGRs it is necessary to characterize the oxidation kinetics, water vapor transport and the development of oxidized layer in candidate graphite grades. It is generally accepted that graphite oxidation by water follows the Langmuir-Hinshelwood (LH) kinetic model. However, oxidation tests performed recently at ORNL on three graphite grades show that the LH model fails to reproduce all experimental data over broad ranges of temperature and concentration. At high water partial pressure (> 200 Pa) and temperatures (> 950 °C) oxidation rates increase faster than the LH model predicts. A LH model modified, that includes a temperature-dependent kinetic order for water vapor modeled as a Boltzmann function, is proposed. The new Boltzmann-enhanced LH model can now consistently reproduce all oxidation rates measured for several graphite grades, and can be used for more reliable prediction of long term evolution of chronic oxidation effects.

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Oscillations in catalytic solid-gas systems

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Catalytic solid-gas reactions are non-linear multilevel chemical reaction systems, which present either steady-state or complex temporal behavior such as instabilities, oscillations, chemical waves or chaos.

The temperature oscillations observed during the oxidation of methanol and ethanol on Pd-Al₂O₃ was registered and considered like a non-isothermal process in which the necessary energy for oscillations was brought not from outside, but from inside, by the exothermic process of oxidation.

Using this type of kinetics the activation energy of both reactions were determined. Several kinetic models, based on Langmuir-Hinshelwood mechanism were also presented.

Characterization of some TiO₂ – HA biocomposites produced by TSS process of the nanosized HA and TiH₂ powdersC. Marinescu¹, A. Sofronia¹, E.M. Anghel¹, O. Gingu² and S. Tanasescu¹

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TiO₂ (titania) reinforced HA (hydroxyapatite) composites were obtained by a two-step sintering (TSS) process of a homogenous mixture of nanosized HA and TiH₂ (titanium hydride) powders. The resulted TiO₂-HA composites are candidates for engineered tissue implants [1]. Structural, spectroscopic, morphological and thermal characterization of the raw powders and TiO₂-HA composites was performed. The results suggested that as the sintering holding time increased from 5h to 10h, a homogenous TiO₂-HA composite (36 % rutile) with smooth surface and a thermal expansion coefficient of $11.46 \cdot 10^{-6} \text{ C}^{-1}$ in the 40 - 1000 °C range was formed. Higher porosity of HA compared to TiO₂ – HA composite indicates the important role of titania particles in lowering surface roughness and densifying composite. One of the major advantage of TSS process over classical sintering one consists in restraining of the HA decomposition and thus avoiding formation of detrimental TCP in the composite. Kinetics and activation thermodynamic parameters (changes of entropy, enthalpy and free Gibbs energy) of TiH₂ dehydrogenation process were obtained.

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Sulfur chemisorption on metal oxides

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Super critical water (SCW) gasification is a promising option in the field of energy harvesting from wet organic streams, such as biomass or wastes. A major issue to be solved is the requirement of an effective conversion within a catalyst mediated process in which the catalyst is extremely sensitive to poisoning already by a few PPMs of sulfur (S) species remaining within the SCW phase. Several approaches exist to overcome the catalyst poisoning by S, but removal by adsorption is the least expensive. Adsorbent material is sought as a metal oxide, in which S is replacing the superficial oxygen and forming stable chemical bonds. This study is aimed to develop an ideal metal oxide which is able to efficiently chemisorb S at SCW conditions. From the thermochemical point of view, the materials have been selected based on the strength of the metal-S chemical bond. The stability under SCW conditions of the chosen metal oxides has been also evaluated.

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Conformer entropy influence on the biological activity of bioactive molecules

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Entropy of 12 PM3, 14 PM6, and 19 PM7 conformers of (3S,5S,6S)-6-acetylamidopenicillanic acid has been calculated. The cubic interpolation relations of functional dependence of enthalpy (ΔH), entropy (ΔS) on temperature ($T \in [200K, 400K]$) were established:

$$\Delta S_{PM3}(T) = 59.6464(\pm 1.8190) + 0.3128(\pm 0.0072)T - 1.9950(\pm 0.1791) \cdot 10^{-4}T^2 + 1.2464(\pm 0.1563) \cdot 10^{-8}T^3$$

$$\Delta S_{PM6}(T) = 59.9525(\pm 2.3171) + 0.3216(\pm 0.0060)T - 2.1817(\pm 0.1463) \cdot 10^{-4}T^2 + 1.4421(\pm 0.1269) \cdot 10^{-8}T^3$$

$$\Delta S_{PM7}(T) = 57.8610(\pm 1.4862) + 0.3182(\pm 0.0046)T - 2.1507(\pm 0.1076) \cdot 10^{-4}T^2 + 1.4039(\pm 0.0920) \cdot 10^{-8}T^3$$

Considering the relation: $\Delta G = \Delta H - T \cdot \Delta S$ we can state that the thermodynamic factor, which determines the variation of the conformers' biological activity, is the entropic factor, which represents the quantity of a bound energy. Based on this observation, the following theorem can be stated: ***The dispersion of biological activities of all conformers at a temperature T is determined by their entropy.***

The measurement and kinetic relevance of the ignition delay time

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Ignition delay time is a helpful characteristic of self-ignition process, frequently employed to rationalize the kinetics of the early stages of combustion. It is frequently measured using either rapid compression machines or shock tubes. Recently, it was shown both theoretically and experimentally that an ignition delay time also exists after a spark discharge in a flammable mixture before the beginning of flame propagation. Numerical studies for spark ignition in quiescent flammable mixtures modeled the ignition and flame propagation using the ignition delay time, defined as the time interval between the start of the energy input and the onset of ignition [1]. On the other hand, the analysis of the early stage of pressure rise in a closed vessel indicated the validity of a third power law, $\Delta P = k_3 \cdot t^3$. Due to inherent displacements of both abscissa and ordinate during the pressure-time recording, an improved correlation equation with three adjustable parameters proved to fit better the experimental data for ΔP lower than initial pressure [2], $\Delta P = a_0 + k_3 \cdot (t - \tau)^3$, where τ is the ignition delay time. The existence of this ignition delay period is confirmed by simultaneous measurements of the emitted radiation from the expanding flame using a photodiode. The obtained curve exhibits a specific pattern during ignition and subsequent propagation. Relevant results are given for various CH₄-air-inert mixtures.

[1] J. Han, H. Yamashita, N. Hayashi, *Combust. Flame*, **2010**, *157*, 1414–1421

[2] D. Razus, D. Oancea, C. Movileanu, *J. Loss Prevent. Proc.*, **2006**, *19*, 334–342

Non-uniform binding and reactivity: from adsorption equilibrium, via single-route complex reactions, to bacterial growth kinetics

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Originating in Taylor’s theory of active centers in heterogeneous catalysis, the problem of surface non-uniformity was developed within the Russian school, with important contributions of Roginskii and Temkin. Further approaches included the so-called “condensation approximation” (CA) initially advanced by Harris and subsequently developed by the Polish school of Rudzinski and Jaroniec. In dealing with adsorption equilibrium the problem reduces to a Fredholm integral equation of the first kind, which bears the inconvenience of the so-called “illposedness”. Approximate solutions are necessary as the elegant analytic one of Sips is limited to a narrow choice of expressing the experimental data. Temkin’s model (TM) of non-uniform reactivity, derived in terms of linear free energy relationships, is a valuable alternative to various “exact” and “approximate” methods.

A review of the author’s contributions in this field is presented. It starts with an improved version of the CA, continues with the critical analysis of TM and the development of an extended version (ETM), a general model of single-route catalytic reactions with non-uniform reactivity, a discussion of structural and kinetic sensitivity within this general model, and finally the application of Boudart’s principles of “simplified kinetics” to bacterial growth kinetics with uniform and non-uniform binding and reactivity.

This work is dedicated to the memory of Professor Eugen Segal who inspired, partially co-authored and was a close and sharp witness to the embodied efforts.

Image furnace floating zone crystal growth: an adventure of several decades

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<http://www.icmмо.u-psud.fr/Labos/SP2M/cv/Pers-Revco.php>

Crystal growth by the floating zone method associated with an “image furnace” is a technique developed and used by the author over five decades in the field of oxides. It has proved to be an extremely fruitful companion of his research and that of his coworkers in many areas of materials science, solid state chemistry and solid state physics.

A brief account of the main results and scientific breakthroughs achieved over the years using the materials or oxide crystals grown by the technique will be given. This review, focusing on a limited number of examples, will browse through bicrystal growth and grain boundary studies, high T_c superconducting oxides work, spin-Peierls and spin-ladder oxide compounds, geometrical magnetic frustration in pyrochlore oxides and recent work on spin-chain oxides which exhibit a remarkable high unidirectional thermal conduction of magnetic origin.

New developments and prospective ideas will be discussed.

**Thermodynamic properties of nanostructured materials:
interplay between thermodynamic stability, synthesis conditions and microstructure**

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Understanding the properties of nanoparticles presents a host of challenging questions and problems. In the present paper we will pay special attention to the role of the energetic parameters in understanding the nanomaterial stability in the view of their applications. Some compounds from two particular systems were selected for discussion: nanostructured multicomponent transition metal oxides and nanoalloys. In the first case, the focus of the research was to emphasize modifications of the thermodynamic properties connected with the changes in the morphology of nanocrystalline barium titanate (BaTiO_3). In the second case, the goal is to investigate the characteristic parameters that favor stable nanostructured phases in Ag-Cu nanoalloys. By determining the correlations between thermodynamic properties, synthesis conditions and different compositional variables, it should be possible to identify the possibilities to control and optimize the materials properties for specific applications.

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Partial molar excess enthalpies at infinite dilution measurements for two prototype ionic liquids in water at 303.15 and 318.15 K*

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In the recent years the ionic liquids (ILs), a new class of green solvents, got an increased importance due to their unique physicochemical properties. Their negligible vapor pressures recommended them as replacements for the highly flammable and toxic volatile organic compounds (VOCs) and in a growing number of applications. The hygroscopic character of the ILs has significant practical consequences. Therefore, the physicochemical properties of the ILs aqueous solutions have to be investigated rigorously. For a better understanding of solution behavior, it is recommended to evaluate the derivative excess properties at infinite dilution, where a single solute molecule is completely surrounded by solvent. Since solute-solute interactions are no longer present, infinite dilution excess properties reflects almost completely unlike pair interactions and yield information about such intermolecular forces. In the present work, enthalpies of solution for 1-butyl-3-methylimidazolium chloride and bromide + water binary systems have been measured by calorimetry in the dilute region at two temperatures. The results are reported in terms of excess molar enthalpies, H_m^E , and molar enthalpies of solution for ILs. The latest data have been used to calculate the values at infinite dilution. The H_m^E data are evaluated by their correlation with the Redlich-Kister equation. Structural effects and physical interactions for the binary systems are discussed by comparison.

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Fluorine adsorption on the modified tripoli. The equilibrium and kinetics.

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The equilibrium and kinetics of fluorine adsorption from the NaF model solution onto the natural tripoli from Senatovka deposit, modified with structural chemical method (hereinafter called TSM) have been studied.

Experiments on the adsorption of fluoride were carried out in batch conditions. The main experimental parameters varied in the following range: the fluorine concentration from 0.10 to 4.75 mmolF / L, ratio S: L = 1.0- 10.0 g/L, pH = 4.5-8.5, the solution temperature was 20, 30, and 40°C. The optimal conditions for the removal of fluoride from water were determined.

TSM adsorption capacity is 4.82 mgF/g at initial fluorine concentration 19.5 mgF/L.

The adsorption isotherms of fluorine obtained for initial and modified samples were simulated using the Langmuir, Freundlich, and BET equations; the parameters of these equations have been calculated. It is shown that the Langmuir model better describes the experimental data of F⁻ adsorption at 20°C.

The kinetic curves of fluorine sorption were obtained at different temperatures. The simulation of the kinetic curves using the kinetic equations of the pseudo first and pseudo second order, Elovich and intraparticle diffusion equations has been carried out. It was shown that the kinetic model of the pseudo-second order better describes the experimental data on the kinetics of fluorine adsorption by modified tripoli sample.

Mechanistic studies on the role of $[\text{Cu}(\text{CO}_3)_n]^{2-2n}$ as a water oxidation catalyst

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Recent interest in the field of water oxidation has triggered the discovery of a wide variety of catalytic systems, homogeneous and heterogeneous. Identification and direct observation of the key intermediates is vital for unraveling the mechanism of water oxidation in a particular system. Recently it was reported that $[\text{Cu}(\text{CO}_3)_n]^{2-2n}$ acts as an electro-catalyst for the oxidation of water. The detailed mechanism was discussed but the question whether a Cu^{III} or a Cu^{IV} intermediate is the key oxidizing agent was not elucidated. Pulse radiolysis is known as a mechanistic tool for elucidating the mechanisms of single-electron redox processes. Under the same conditions described in the electro-catalytic study pulse radiolysis measurements revealed that $[\text{Cu}^{\text{III}}(\text{CO}_3)_n]^{3-2n}$ has a spectrum similar to that observed electrochemically. Furthermore the kinetics of disappearance of $[\text{Cu}^{\text{III}}(\text{CO}_3)_n]^{3-2n}$ obey a second order rate law. DFT calculations reveal a significant charge transfer from the coordinated carbonate to $\text{Cu}(\text{III})$, suggesting that the coordinated carbonate has a radical character.

SECTION 2

Chemical kinetics and thermodynamics

POSTERS

**Thermodynamic stability of the $\text{Ba}_x\text{Sr}_{1-x}\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$
($x = 0.2, 0.4, 0.5, 0.6, 0.8$; $y = 0.2, 0.8, 1$) perovskite-type oxides**

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For a better understanding of the stability limits of the perovskite phases in mixed electronic/ionic conducting oxides, a set of experiments concerning the thermodynamics of the perovskite-type oxides $\text{Ba}_x\text{Sr}_{1-x}\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$ ($x = 0.2, 0.4, 0.5, 0.6, 0.8$; $y = 0.2, 0.8, 1$) (BSCF) was initiated. New features related to the influence of the dopants and oxygen nonstoichiometry on the thermodynamic behavior was evidenced. The partial molar free energies, enthalpies and entropies of the oxygen dissolution, and the partial pressures of oxygen have been investigated using solid state electromotive force measurements, the measurements being performed in the temperature range of 873-1273 K and at 10^{-7} atm surrounding atmosphere. This study attests the phase instability of BSCF during heating at temperatures lower than 1123 K. The temperature of structural transformations related to the charge compensation of the material system was evidenced.

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**Modeling the conformational characteristics
of ionic polymers in solution induced by the presence of polyvinyl alcohol**

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Ionic polymers represent a class of chemical compounds which have gained a great interest in various scientific fields, so that, the study of polyelectrolytes solution dynamics is necessary to gain insight into biomedical or industrial processes. The cationic polysulfones containing quaternary ammonium side groups (PSFQ) was recommended for such applications due to their special solution properties. These properties can be optimized by blending of PSFQ with other synthetic polymers (*e.g.*, polyvinyl alcohol, PVA). Thus, present study performed in dilute solution is based on researches concerning the viscometric and conductometric behavior of PSFQ/PVA mixture in N-methyl-2-pyrrolidone (NMP), and competition between different types of interactions occurring in system. The results have shown that the addition of PVA at PSFQ solution leads to a decrease of the specific viscosity and implicitly, of the conductivity as results of his higher flexibility. Thus, the modification of polymer blends composition leads to conformational changes of polymer chains in ternary system. This trend of macromolecular chains rearrangements in dilute solution are generated by interactions which will dictate the specific characteristics of corresponding membranes predestined for specific applications.

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Physicochemical properties for some heavy alkane with alkylbenzenes binary mixtures at different temperatures up to 318.15 KD. Drăgoescu¹, F. Sîrbu¹, A. M. Popescu¹, V. Constantin¹, A. Shchamaliou² and T. Khasanshin²¹„Ilie Murgulescu” Institute of Physical Chemistry, Romanian Academy,
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The physicochemical properties for the binary mixtures of n-hexadecane with two isomers of benzene, as tert-butylbenzene and isoproylbenzene, were measured at several temperatures in the range of (298.15 to 318.15) K and atmospheric pressure. Densities, speeds of sound, refractive indices, at temperature of $T = 318.15$ K, and electrical conductivities at five temperatures between (298.15 and 318.15) K are reported. From the obtained experimental results, the isentropic compressibilities, the excess isentropic compressibilities, the deviation in refractive indices and the molar refractions were calculated. The excess properties were fitted to the Redlich-Kister type polynomials. The experimental and calculated results are discussed in terms of molecular interactions and structural effects between components of mixtures.

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**Quaternized polysulfone/polyvinyl alcohol multicomponent system:
Computational modeling of hydrogen bonding and electrostatic interactions**

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Functionalized polysulfones present interesting properties that led to a wide spectrum of applications. The ability of quaternized polysulfones (PSFQ) to act as the integral medium of biological is enhanced by blending with a suitable hydrophilic additive (*e.g.*, polyvinyl alcohol, PVA). It is found that dynamics of PSFQ/PVA mixture in N-methyl-2-pyrrolidone (NMP) vary with thermodynamic balance between flexibility and structural stability, determined in the chemical and physical responses of polymers to cumulative effects of the electrostatic interactions and hydrogen bonding. This provides insight into the general concept of solution dynamics of polymer mixtures and is discussed based the computational chemistry and mathematical simulations. In this context, the specific inter- and intramolecular interactions established in PSFQ/PVA/NMP system, with proton – donor and/or proton – acceptor properties, were evaluated through the mathematical simulations, being corrected on the basis the association/interaction constants, imposed by the occurrence of the associated species, as a function of the system composition. Investigation of the thermodynamic functions from the perspective of new theories is useful in the optimal choice of polymer mixtures composition for specific applications in the biomedical field.

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The calorimetric study of L-, D- and DL histidine isomers

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The present study aims the experimental determination of the thermochemical properties of histidine enantiomers (L- and D-) and of their racemic mixture and of the thermal behavior including obtaining the parameters characterizing the transitions. The combustion and formation enthalpies corresponding to the crystalline state of compounds were obtained and information concerning their stability obtained by correlating the values of the above thermochemical quantities with the structure of the molecules by using the additivity schemes. The values of the formation enthalpies highlight the stability of the compounds. The thermal behavior of histidine isomers was investigated by means of DSC in the temperature range between ambient and melting-decomposition temperatures. The decomposition mechanism is discussed in correlation with the data obtained by means of DSC.

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Structure and kinetics of *Candida Rugosa* lipase encapsulated in reverse micelles

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The enzyme stability is an important task of research. This study is focused on the effect of trehalose, myo-inositol and phytic acid on the structural stability and kinetics of *Candida Rugosa* lipase encapsulated in reverse micelles. Spectroscopic insights were revealed on the structure of lipase using UV-Vis, steady-state fluorescence and circular dichroism. The kinetics of lipase-catalyzed hydrolysis of olive oil in reverse micellar media in the presence of osmolytes was studied. The fluorescence results show that the structure of lipase is modified by osmolytes in aqueous and micellar media. Circular dichroic spectra indicated that the protein undergoes conformational changes upon interacting with these osmolytes. The kinetics of the enzyme encapsulated in reverse micelles in the presence of trehalose, myo-inositol and phytic acid differ from those when none of the additives were present. Lipase exhibits "superactivity" in reverse micelles when trehalose and myo-inositol are present and the activity is significantly lowered by the phytic acid. Results of this study could give further insights about the enzyme stabilization mechanism.

Solid state study on inclusion complex formation of 2-hydroxypropyl- β -cyclodextrin with four new thioureides

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The new synthesized 2-thiophene carboxylic acid thioureides: N-(p-methoxyphenyl)-N'-(2-thenoil)-thiourea (I), N-(p-methylphenyl)-N'-(2-thienyl)-thiourea (II), N-(p-methylphenyl)-N'-(2-thenoil)-thiourea (III) and N-(p-methylphenyl)-N'-(3-thenoil)-thiourea (IV) come to offer significant advantages in future antibacterial treatment strategies. 2-hydroxypropyl- β -cyclodextrin (HP- β -CD) is the most widely used modified cyclodextrin in formulation of drug products. The biocompatibility and inclusion capability of HP- β -CD make it attractive to improve the physico-chemical properties and also the pharmacological effects of hydrophobic thioureides (I), (II), (III) and (IV). In this work, the solid state inclusion compounds between HP- β -CD and thioureides (I), (II), (III) and (IV) with two different molar ratio (HP- β -CD: thioureide = 1:1 and 2:1) were obtained by both physical mixing and co-precipitation methods. The solid powders of pure substances and HP- β -CD/thioureide - complexes were investigated by differential scanning calorimetry, thermogravimetry and scanning electron microscopy methods. The thermal behavior of the samples well correlates with the observed morphology. The results showed that not only 1:1, but also stable 2:1 inclusion complexes can be formed between HP- β -CD and thioureides (I), (II), (III) and (IV) and the 2:1 host:guest molar ratio of complexes show a properly fitting of drug with two HP- β -CD molecules.

The effect of calcium fructoborate on some organic components of human cerebrospinal fluid

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Cerebrospinal fluid (CSF) is in direct contact with the brain and spine and CSF analysis is more effective than other tests for understanding central nervous system symptoms. The introduction of foreign substances in CSF significantly impedes the normal drainage of CSF thus, acute and chronic pathological changes may occur. FBCa is a natural sugar-borate ester which has nutritional properties and therapeutic potential. Recent scientific papers highlighted the advantages of using FBCa as bioadhesive in prosthesis manufacture, also as an osteoinductive factor with large tissues compatibility and anti-inflammatory effects. In the usual situation of the cranioplasty prosthesis production, the knowing of FBCa interaction with CSF components is an essential issue. In this work, calorimetry, UV-Vis spectroscopy, dynamic light scattering methods and pH measurements were used in order to characterize the interaction between FBCa and CSF components: albumin and natural amino acids tryptophan, histidine, tyrosine and arginine. The obtained thermodynamic parameters and binding constants are suitable criteria in order to express the biocompatibility of FBCa and the significance of the results in this work can be extended to numerous fields that involve the study of the medical formulations.

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Thermodynamic study on host-guest interaction of doxorubicin with β -cyclodextrin and γ -cyclodextrin

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The purpose of this study was to improve the thermal stability of doxorubicin (Dox) by complexing with beta-cyclodextrin (β -CD) and gamma-cyclodextrin (γ -CD). Cyclodextrin (CD) complexes are widely used in the pharmaceutical field and β -CD and γ -CD are the least toxic cyclodextrins for the human body. Dox is a drug available for treatment of different types of cancer which can be used individually or in combination with other chemotherapeutics. A comparative study of β -CD/Dox and γ -CD/Dox binary systems was performed both in aqueous solution (using isothermal titration calorimetry - ITC) and in the solid state (using differential scanning calorimetry - DSC) and thermogravimetry - TG). The solid inclusion compounds were prepared in 1:1 molar ratio of the host and guest using "melting in solution" method. The DSC/TG data of the solid β -CD/Dox and γ -CD/Dox were carried out over a temperature range of 25 – 500 °C at a heating rate of 10 °C/min and the results suggest that the γ -CD/Dox system is thermally stable more than β -CD/Dox system. By means of ITC, the stoichiometric composition, stability constant and thermodynamic parameters of γ -CD/Dox supramolecular structure formation were calculated. It was proved that a 1:1 inclusion complex is formed in aqueous solution for γ -CD/Dox system.

Effect of macromolecules on the aggregation of nano-sized rutile-titanium dioxide

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To produce nano-sized titanium dioxide (TiO_2) coatings, it is desirable that the nanoparticles (NPs) are dispersed into a liquid solution, remaining stable for a certain period of time. Controlling the dispersion and aggregation of the TiO_2 NPs is crucial to exploit their advantages. In this work, 2-hydroxypropyl- β -cyclodextrin (HP- β -CD) and human serum albumin (HSA) solid powders were added separately to the TiO_2 NPs suspensions and the mixture was stirred at room temperature. Once the macromolecules adsorbed onto the NPs surface, the TiO_2 /HP- β -CD NPs and TiO_2 /HSA NPs were collected by centrifugation to remove the unadsorbed macromolecule. Considering the physiological temperature domain, UV-Vis spectra, zeta potential and particle size distributions measurements were done for establish the stability of the NPs based on nano-sized TiO_2 core and a macromolecular shell. Also, solid powder of TiO_2 was characterized by scanning electron microscopy, X-ray diffraction and BET method. The mean hydrodynamic diameter of the TiO_2 /HSA NPs was between 100 nm and 600 nm whatever the initial concentration of HSA. The zeta potential measurements showed that the negative charge of HSA was partially shielded when it was adsorbed at the TiO_2 surface and the TiO_2 /HSA system is dominated by electric double layer interactions. The resulted data reveal that the adsorbed amount of HP- β -CD increases with the initial quantity of TiO_2 and the TiO_2 /HP- β -CD system exhibited a spherical shape and a core-corona structure.

Experimental approaches to evaluate the interaction of cinchonine with β - and 2-hydroxypropyl- β -cyclodextrins

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Cinchonine (Cin) is an alkaloid widely used in pharmacology and in organic chemistry. However, it is poorly soluble in aqueous solutions and is a highly photosensitive compound. An alternative method to improve its physicochemical properties can be the encapsulation by cyclodextrins (CDs). Complexation of Cin with β -cyclodextrin (β -CD) or 2-hydroxypropyl- β -cyclodextrin (HP- β -CD) has been evaluated in 50% (v/v) ethanol – water mixture. The technique employed in solution to determine the stoichiometry and apparent stability constant of the Cin/ β -CD and Cin/HP- β -CD complexes was UV-Vis spectroscopy. The stoichiometry of 2:1 (host:guest) of the complexes was confirmed by Job's plot. The apparent stability constant for the inclusion of Cin with β -CD or HP- β -CD was evaluated at different temperatures using Benesi-Hildebrand method. The values of the thermodynamic parameters ΔH^0 , ΔS^0 and ΔG^0 for the inclusion process were calculated by using Van't Hoff plot. For Cin/ β -CD and Cin/HP- β -CD complexes, the inclusion process is favored through entropy and enthalpy changes. Refractive index, hydrodynamic diameter, zeta potential and pH measurements were done to characterize the association between Cin and considered CDs. Also, complexation of Cin with β -CD and HP- β -CD was studied by isothermal titration calorimetry.

Effect of chain length of alcohols on physico-chemical properties of their binary mixture with halogenated thiourea derivatives

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In the present work, some aliphatic alcohols, namely methanol, ethanol, propan-1-ol, butan-1-ol, hexan-1-ol, octan-1-ol, decan-1-ol and dodecan-1-ol were selected in mixtures with each of the new synthesized thiourea derivatives N-(p-chlorophenyl)-N'-(2-thenoyl)-thiourea, N-(p-bromophenyl)-N'-(2-thenoyl)-thiourea, N-(p-iodophenyl)-N'-(2-thenoyl)-thiourea. These new thiourea derivatives were found to present antimicrobial actions [1]. The characterization of the alcohol/thiourea derivatives binary systems included the determination of refractive index, hydrodynamic diameter, Fourier transform infrared spectroscopy and zeta potential measurements. Also, the UV-Vis absorbance spectra at 25°C for each of the studied systems were recorded. The effect of the different chain length of alcohols on the physico-chemical properties of the binary mixture was analyzed and the resulted data show significant difference between the systems. The importance of analyzing these alcohol/thiourea mixtures is of great interest because of their potential applications in pharmaceutics and it could serve as a reference point for studies of more complex systems.

Reference: [1] C. D. Badiceanu, Al. V. Missir, M. C. Chifiriuc, O. Dracea, I. Raut, C. Larion, L. M. Ditu, G. Mihaescu, Rom. Biotech. Lett., 15 (2010), 5545.

Ignition and propagation properties of coal dust-methane-air hybrid mixtures

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The presence of a flammable gas in a combustible dust cloud significantly modifies its explosivity parameters. Thus, a hybrid mixture can become flammable even when both the dust-air and gas-air binary mixtures are under the corresponding minimum flammable concentrations. The pressure-time histories of hybrid mixtures formed by coal dust, methane and air at different concentrations, at 1 bar initial pressure and normal temperature, were studied using the standard 20 L spherical explosion vessel and both 5kJ chemical igniters and 10 J permanent sparks. From the early stages of the pressure-time history, when the pressure increase is equal to or less than the initial pressure, the normal burning velocities were evaluated and discussed.

Modulation of radiation-induced inactivation of catalase

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The protection of catalase against the γ radiation-induced inactivation is one of key issue that should be addressed during fruit and vegetable processing; therefore, in this study it was aimed the influence of several non-harmful additives such as sodium chloride, propane-1,2,3-triol and sucrose on the stability of catalase during γ -rays irradiation. The structural changes inherent to enzyme inactivation were monitored through the analysis of the ultraviolet-visible (UV-Vis) and circular dichroism (CD) spectra. The effects of the main products of water radiolysis (superoxide anion, hydroxyl and peroxy radicals) on the inactivation degree were studied in the presence of superoxide dismutase (SOD), a radical trapping enzyme. Since no significant changes occurred in the UV-Vis and CD spectra of catalase after irradiation with γ -rays in the presence of modulators, it may be assumed that catalase is inactivated through the radicalic attack of the reactive oxygen species generated during the water radiolysis. This hypothesis is supported by data showing a significant decrease of the inactivation degree in the presence of SOD, confirming the fact that the inactivation occurs mainly via the radical transfer to the active site of catalase.

Overall kinetic parameters of methane oxidation in O₂- or N₂O-supported flamesD. Razus¹, C. Movileanu¹, M. Mitu¹, V. Giurcan¹ and D. Oancea²¹„Ilie Murgulescu” Institute of Physical Chemistry, 202 Spl. Independentei, 060021 Bucharest, Romania²University of Bucharest, Department of Physical Chemistry, 4-12 Elisabeta Blvd., 030018 Bucharest, Romania

The burning velocity is an essential parameter characteristic for flame propagation in deflagration regime, directly influenced by the reaction rate in the flame front. In the present contribution, the burning velocities of the stoichiometric methane-air and methane-nitrous oxide mixtures were determined at various initial pressures between 0.3 and 1.8 bar and ambient initial temperature, under various inert gas (He, Ar, N₂ or CO₂) concentrations. The burning velocities were obtained both from experimental measurements of pressure variation during closed vessel explosions and from the detailed modeling of free laminar premixed flames. For all systems, the temperature profiles across the flame front and the concentration profiles of most important chemical species were examined versus similar data characteristic to lean- and rich methane-oxidizer mixtures. Examination of burning velocity variation against average flame temperature in experiments at constant initial pressure and various inert concentrations allowed the determination of the overall activation energy; examination of the pressure dependence of burning velocity, at constant inert concentration, allowed the determination of overall reaction orders.

**Spherical expanding flames in CH₄ - N₂O - N₂ mixtures:
Laminar burning velocity measurements and kinetic modeling**D. Razus¹, M. Mitu¹, V. Giurcan¹, C. Movileanu¹ and D. Oancea²¹„Ilie Murgulescu” Institute of Physical Chemistry, 202 Spl. Independentei, 060021 Bucharest, Romania²University of Bucharest, Department of Physical Chemistry, 4-12 Elisabeta Blvd., 030018 Bucharest, Romania

The flame propagation in nitrogen-diluted CH₄ - N₂O mixtures was monitored by pressure measurements during explosions in a closed vessel with central ignition. The burning velocity, characteristic for the laminar propagation regime, was calculated from the cubic law coefficients of pressure rise, determined in the early stage of flame propagation by means of a recently developed model. Lean- and stoichiometric methane-nitrous oxide mixtures (equivalence ratios: 0.8 and 1.0) diluted by various amounts of nitrogen within 40 and 60 vol% were studied, at ambient initial pressure and temperature. The burning velocities of CH₄ - N₂O - N₂ mixtures derived from experimental data are examined against computed values, obtained with the package COSILAB for free laminar premixed flames. The kinetic modeling used the GRI-Mech reaction mechanism, developed by the Gas Research Institute-USA for natural gas-air flames in various conditions by taking into account 325 elementary chemical reactions and 53 species. The most important elementary reactions in lean and stoichiometric CH₄ - N₂O - N₂ mixtures were identified by means of sensitivity analysis.

Correlation between thermodynamic properties, microstructure and electrical conductivity of the $\text{Ba}_{0.75}\text{Sr}_{0.25}\text{TiO}_3$ nanopowders obtained by hydrothermal synthesis

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Nanostructured perovskite material $\text{Ba}_{0.75}\text{Sr}_{0.25}\text{TiO}_3$ was synthesized in one step process by hydrothermal method. The microstructure, phase composition and the crystallite size of the perovskite nanopowders have been determined by XRD, RAMAN and SEM analysis. The thermodynamic properties obtained by a couple of measurements in both isothermal and dynamic regimes (drop calorimetry, differential scanning calorimetry, solid-oxide electrolyte galvanic cells method) allow for the investigations of the thermodynamic stability in a large temperature range from room temperature to 1273 K. The correlation of the thermodynamic properties with thermal expansion and electrical conductivity has been investigated. The results are discussed based on the strong correlation between the energetic parameters and the charge compensation of the material system.

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Thermal stability of some perovskite structures obtained by hydrothermal synthesis

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Nanostructured barium strontium titanate (BST) and barium zirconate (BZ) were synthesized in hydrothermal conditions, in one step processes. The chemical properties, the microstructure, phase composition and the crystallite size have been determined by ICP-OES, SEM and XRD. The thermodynamic stability in a large temperature range from room temperature to 1100 °C was investigated in a dynamic regime using Differential Scanning Calorimetry. A comparison from the point of view of thermal stability was done between the two types of perovskites. The BST and BZ samples were then treated at 800 °C and 1000 °C in air vacuum. A comparison between the as prepared samples and the thermal treated ones was also performed from the point of view of thermal stability.

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Thermodynamic behavior at different temperatures on derived compounds from halogenated thiourea in alcoholic solutions with pharmaceutical applications

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Thermodynamic data behavior of halogenated thiourea derived compounds with pharmaceutical important applications [1] has been studied over the whole molar concentration range of N-(p-iodophenyl)-N'-(2-thenoyl)-thiourea and alcoholic aqueous solution in ternary liquids mixtures. Density, speed of sound and refractive index were measured at molarities between $(0.5 \text{ and } 1.05) \cdot 10^{-5} \text{ mol} \cdot \text{dm}^{-3}$ range in 50 % ethylic alcohol solutions at the seven temperatures from (288.15 up to 318.15) K and at atmospheric pressure. The derived thermophysical properties for halogenated thiourea derived compound in ethylic alcohol have been determined using experimental results. The apparent molar volumes, standard apparent partial molar volumes at infinite-dilution from N-(p-iodophenyl)-N'-(2-thenoyl)-thiourea to alcoholic solutions, isentropic compressibility coefficient, the standard partial molar isentropic compressibility have been calculated, and the refractive indices data were evaluated using Lorentz-Lorenz equation. The correlations among different thermodynamic properties [2,3] were represented.

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Thermokinetic and thermodynamic parameters of the titanium hydride dehydrogenation process

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Titanium is known to have a large affinity for hydrogen. Hydrogenation can lead to the formation of titanium hydrides which present different stoichiometries [1]. TiH₂ is used in applications as pyrotechnic and metallurgical areas, hydrogen storage media and as brazing aids in sealing ceramics to metals, etc [1]. Kinetics of TiH₂ dehydrogenation process is not clear at present and needs further investigation. Thermal behavior of TiH₂ powder at heating was studied by means of thermogravimetry and differential scanning calorimetry in the 25 – 900 °C range. The results show the nonisothermal dehydrogenation occurred in a three-step process. The maximum rate of decomposition at 579°C corresponds to a sharp peak on the DTG curve. The TG curve showed the gain in weight because of the slight oxidation above 606°C. Kissinger equation was employed to obtain kinetics parameters of the process. The activation enthalpies of transformation corresponding to the three-step process are: 190.73±0.091, 153.82±0.122 and 114.48±0.185, respectively.

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Thermodynamics of nanoparticles-protein interaction: the effect of TiO₂ and ZnO nanoparticles on the thermodynamic stability of bovine serum albumin

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The thermodynamics of protein-nanoparticle interaction is a key issue for nanosafety research. In the present study, the effect of two of the most commonly used metal oxide nanoparticles (NPs) - zinc oxide (ZnO) and titanium dioxide (TiO₂) - on the thermal stability of bovine serum albumin (BSA) has been investigated. Phosphate buffer - dispersed NPs with different concentrations were prepared and interaction with the protein was evidenced by using the NanoDSC (TA Instruments) equipment: a clear altering of the thermal behavior of BSA in phosphate buffer at different pH values, in both free state and bound to the NPs has been observed. The thermodynamic parameters of the thermal fingerprint of the protein, represented by denaturation temperature (T_m) and heat capacity (ΔC_p), enthalpy (ΔH), entropy (ΔS) and free energy (ΔG) changes have been evaluated. Calorimetric data clearly indicate severe structural rearrangements of BSA bound to NPs. The shape of the unfolding thermograms also revealed the nonuniform character of the protein population due to the surrounding buffer.

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Excess thermodynamic properties for a prototype ionic liquid + 1-butanol binary system at low pressures and several temperatures*

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Experimental isothermal vapour-liquid equilibrium (VLE) data are reported for the binary mixture containing 1-butyl-3-methylimidazolium chloride ([bmim]Cl) + 1-butanol at three temperatures: (353.15, 363.15, 373.15) K, in the range of 0-0.17 liquid mole fraction of [bmim]Cl. Excess molar Gibbs energy, G_m^E and activity coefficients of the two components, γ_i , have been evaluated. Additionally, refractive index measurements have been performed at three temperatures: 298.15, 308.15 and 318.15 K in the whole composition range. Densities, excess molar volumes, surface tensions and surface tension deviations of the binary mixture were predicted by Lorentz-Lorentz (n_D - ρ) mixing rule as well as dielectric permittivities and their deviations by known equations. Enthalpies of solution for [bmim]Cl + 1-butanol system have been measured over the composition range of 0.0006 to 0.0793 mole fraction of [bmim]Cl at temperatures of 303.15, 310.43 and 318.15 K. These results are reported in terms of excess molar enthalpies, H_m^E , and molar enthalpies of solution for [bmim]Cl. The latest data have been used to calculate molar enthalpies of solution for solute at infinite dilution. All types of experimental data were correlated using the Redlich-Kister model. Based on excess thermodynamic properties, structural effects and physical interactions for the binary system are discussed.

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Simulations of experimental air-methane explosionsN.I. Vlasin¹, M. Prodan², E. Ghiciei³ and D. Chirila⁴

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Mostly, the validation of computational simulations is performed based on physical experiments. In the case of gas explosion, the experiments are carried out in the pressure resistant vessels that do not allow imagery analysis of the phenomenon. To counteract this impediment, it was built an experimental stand consists of a transparent tube and of special equipment for visualization the flame front by Schlieren effect, thus enabling the high speed records of the flame behavior in fast combustions of air-methane mixtures. The high speed video recordings were then contributed to calibrate the computer simulations of air-methane explosions, their validation being not necessary once the experiment's results are consistent with those obtained in the virtual environment.

SECTION 3

Functional Interfaces. Aquaculture and food applications.

KEYNOTES

Romanian Center for Recirculating System Modelling and future of Danube sturgeons

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In Romania, in the last years, many researches dealt with sturgeon aquaculture in the way of maximizing production efficiency (highest growth and survival rates), improving reproduction technologies and quality of the sturgeon products obtained from new emerging intensive production systems like recirculating systems. Besides providing a consistent supply without exploiting them, sturgeon aquaculture can also help for the conservation of declined wild populations through restocking. The main aim of researches regarding sturgeon restocking is to improve fitness for survival in the wild.

In order to overcome the fast decline of sturgeon's population, the aquaculture technologies for reproduction and fry rearing for both purposes (rearing and restocking) must be though enhanced. Thus, through a multidisciplinary experimental approach, the Romanian Center for Recirculating System Modelling established by University “Dunarea de Jos” of Galati as a results of implementing an infrastructure modernization project founded by POSCCE program enables complex testing solutions in order to develop methods and new technologies which will underpin the aquaculture competitiveness, both scientifically and socio-economically, contributing therewith to the better understanding of sturgeon biology and behavior in the wild. The main aim of the present paper is to synthesize the research achievements and identify research approaches and strategies to secure the future of Danube sturgeons.

Effect of interface on the biomimetic reconstruction of enamel-type biomaterials in the presence of different hydrogel bioactive templates

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The biomimetic synthesis of enamel-like biomaterials is of great interest in tissue engineering, as a bottom-up remineralizing strategy. The paper presents a comparative study on the in vitro biomimetic remineralization of the tooth components layers (enamel, dentine and) using chitosan-enamel matrix derivative(EMD)-calcium chloride hydrogel as biomimetic precursor, by incubation in a phosphate solution containing fluoride, at 37 °C for 2-10 days. As EMD template we used both commercial Emdogain gel matrix proteins premixed with propylene glycol alginate or agarose polysaccharide precursor.

The effect of interface chemical composition (organic vs. inorganic preponderantly biosubstrates and proteins-based vs. polysaccharides-based hydrogel precursors), morphology (defects generated by acid-etching of biomaterial surface) and interfacial tension on the hydroxyapatite nucleation, orientation, crystallite size and composition inside the grown mineralized layer was studied by scanning electron microscopy coupled with energy dispersive x-ray spectrometry (SEM-EDS), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy and X-ray diffraction (XRD). The effect of chitosan on the above mentioned characteristics of the obtained remineralized layers was investigated.

A review: Heavy metals concentration in fish meat from the Danube River

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Issues regarding water pollution with heavy metals increased its scale of interest among researches, fact that is justified by the global upward tendency of heavy industry. In Romania, Danube River is categorized as the most important river from the economical point of view, both for its navigation route and consistent and valuable fish stocks. Several studies have emphasized the problems related to high environment pollution, especially with heavy metals, in the Danube ecosystems. The current paper aims to present information regarding the heavy metals accumulation in fish from the Danube River. Various databases were revised and the relevant information was centralized, in order to obtain a clear view on the concentration dynamics and accumulation tendency of several heavy metals, as follows: Cd, Pb, Hg, Cu and Fe. As a conclusion to this research, it can be stated that the maximum Cd, Pb, Cu and Fe concentrations were reported as being found in *Alosa pontica* at 863 river kilometer (0.433 $\mu\text{g/g}$ DW) for Cd, 257 river kilometer (0.65 $\mu\text{g/g}$ DW) for Pb, 257 river kilometer (5.34 $\mu\text{g/g}$ DW) for Cu and respectively, 863 river kilometer (40.36 $\mu\text{g/g}$ DW) for Fe. Regarding mercury, the maximum concentration was reported as being found in *Sander lucioperca* at 1168-1170 river kilometers (1.32 $\mu\text{g/g}$ DW).

The influence of water and sediments nitrite concentration on chemical fish meat composition in different aquatic ecosystems

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Pollution is a worldwide issue nowadays, fact that makes food safety a very popular concept that is encountered among the latest research in food chemistry field. The aim of the present study is to evaluate the chemical fish meat composition in terms of nitrites, in different ecosystems, in correlation with the concentration of nitrites from water and sediments. Therefore, samples of water, sediments and fish were collected from the following areas: Black Sea – Perisor (44°47'59.2"N - 29°16'14"E), Black Sea – Sfântul Gheorghe (44°52'51.3"N - 29°37'18.8"E), Danube Delta - Soschi Lake (44°58'43"N - 29°10'55"E), Danube Delta - Barcaz Lake (44°58'24"N - 29°12'54"E), Danube - Tulcea Port (45°10'53"N - 28°47'34"E), Danube – Galati Port (45°25'44"N - 28°3'25"E), Petrei Lake and Pond (43°3'9"N - 29°7'49"E), Malina Lake and Pond (45°24'27"N - 27°57'13"E) and also a recirculating aquaculture system (RAS) and a recirculating aquaponic integrated system (RAIS). In Danube - Tulcea Port (0.2468mg/L), Danube – Galati Port (0.2083mg/L) and Black Sea – Sfântul Gheorghe (0.1988mg/L) were registered the highest concentration of nitrites in water, fact that generates a direct statistically significant correlation with the concentration of nitrites from fish meat and sediments, recorded in those studied areas. Thus, it has been concluded that there is a strong direct correlations between nitrites concentration in fish meat, sediments and water. However, the obtained data shows no food safety concerns, since all the nitrite concentrations recorded in fish meat are below the maximum limit for human consumption.

Danube sturgeons - Current status and conservation measuresRadu Suciu¹, Tudor Ionescu², Victor Cristea² and Iulian Birsan²¹Danube Delta National Institute, Tulcea, radu.suciu@ddni.ro²Lower Danube University, Galatz

Only five out of six former existing species of sturgeons still survive in the Danube River but only three long-migratory and one resident freshwater species (sterlet) continue to spawn in the Lower Danube River. Following a period of 10 years (1990 - 2000) of unregulated and uncontrolled fishing, despite regulations adopted in year 2001 and five years of implementation of regulations adopted by the Convention on International Trade in Endangered Species of Wild Fauna and Flora (CITES), stocks of sturgeon populations were declining dramatically. Romanian authorities for environment and agriculture adopted in May 2006 a ten year moratorium on commercial catches of sturgeons and started to implement on annual basis (2006 - 2019) supportive stocking of the river using young sturgeons obtained by controlled propagation of wild brood stock captured in the river. In year 2010, due to financial shortages and the impossibility to conduct comprehensive evaluation of the stocking procedures and results, the supportive stocking programme was discontinued. The Lower Danube University of Galatz started in year 2013 a large scale in situ pilot project, funded by the Romanian Fishery Operational Programme (FOP), to evaluate the survival and distribution of young sturgeons stocked experimentally in different locations of the Lower Danube River. The main results of the evaluation were that young sturgeons stocked in the river adapt well to feed and grow well in the wild environment. Continuation of the commercial catch moratorium for the next 5 years (2016 - 2020) was adopted by a regional meeting of CITES and fishery authorities held in Bucharest in November 2015.

SECTION 3

Functional Interfaces. Aquaculture and food applications.

POSTERS

Water Quality Monitoring into a Recirculating Aquaculture System

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Abstract text. Aquaculture is the fastest growing food-producing sector, accounting about nearly 50% from the total fish production of the world. Due to this rapid increase and to the environmental constraints (environmental pollution, limited water resources, high costs associated with land and water), the producers were forced to develop new facilities in order to sustain the consumers demands. Thus, in last years, the intensive and super-intensive aquaculture has developed particularly among recirculating systems (RAS), where environmental conditions are permanently monitored and controlled, and the water requirements are quite low because the water is reused in the production. Moreover, the practice of the last decades indicates that RAS production is a feasible alternative to traditional pond aquaculture. In this context, the purpose of this study was to monitor the water quality in a recirculating aquaculture system for growing of *Acipenser gueldenstaedtii*, taking into consideration the demands of the fish for oxygen, temperature, pH, ammonia, nitrite (NO₂), nitrate (NO₃), turbidity, conductivity, total dissolved solids (TDS) and total suspended solids (TSS). The experiment was conducted in Galați, at the Romanian Center for the Modeling of Recirculating Aquaculture Systems (MORAS), facilities of University Dunărea de Jos, Romania and lasted for 4 weeks.

Novel biosensor based on L-amino-acid oxidase and polypyrrole for detection of L-Tyrosine in pharmaceuticals

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This work describes the developing and optimization of a novel biosensor for the quantification of L-amino acids present in pharmaceutical samples. The receptor element of the biosensor is developed from a platinum electrode modified with polypyrrole doped with Prussian blue and L-amino-acid oxidase. Biosensing target molecule is the hydrogen peroxide formed in the enzymatic process catalyzed by the L-amino-acid oxidase immobilized onto polypyrrole matrix. Detection technique was fixed potential amperometry. The optimizations of supporting electrolyte properties and of detection technique parameters were carried out. Assessment of the biosensor capacity to detect different L-amino acids demonstrate higher sensitivity for L-tyrosine. For the L-tyrosine detection a low limit of detection of 5.3×10^{-7} M and a wide linearity range between 1×10^{-6} and 2×10^{-4} M were achieved. The interferences were studied by standard addition method obtaining an excellent average recovery of 99.84%. The validation was carried out by quantification of L-tyrosine in pharmaceutical samples and the values compared with standard reference method.

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Chemical sensors applied in the analysis of pharmaceutical products

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Chemical sensors could have multiple applications in the analysis of pharmaceutical products, both qualitative analysis and quantitative analysis. Chemical sensors developed in this study, based on carbon modified with cobalt phthalocyanine or Meldola's blue, were used to analyze various commercial formulations of ibuprofen. Electrochemical signals obtained by cyclic voltammetry are related to electroactive compounds from the sensing element, to ibuprofen from the solution and interactions between both processes. In optimal conditions, there were determined the analytical properties of sensors. Linearity range of dependence of the most intense peak current from the cyclic voltammogram and the analyte concentration was ranging from 5 to 600 μM . The detection limits were between 1.45 and 2.32 μM . Interferences of excipients in the determination of ibuprofen are below 1%. The analytical method based on chemical sensors was compared with the UV spectrophotometric method yielding correlation coefficients of greater than 0.96.

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Spectroelectrochemical characterization of pyrrole polymerization *in situ* with selected fungal strains

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Polypyrrole (PPy) is one of the most studied amongst conductive polymers. Its employment in medical fields such as biosensors, drug delivery devices and bio-actuators has increased the interest towards synthesis routes that overcome biocompatibility issues associated with traditional methods for polymerisation (i.e. chemical, electrochemical). Biocatalytic polymerizations have been widely investigated as a reliable and environmentally friendly option. Due to the fact that enzyme purification represents a costly and time-consuming procedure, whole cells provide an efficient alternative for biocatalysis since enzymes are usually more stable in their natural environment.

Some fungal strains have been studied and selected according to their ability to induce the synthesis of polypyrrole micro-particles *in situ* under controlled submerged fermentation conditions. The polymerization process was recorded for the most performant strains.

UV-Vis spectroscopy was employed to monitor and characterize the biocatalysis process revealing the formation of polypyrrole along with cyclic voltammetry for investigating the redox behaviour of the samples. SEM microscopy was applied for morphological characterization of the polymer micro-particles.

Electrokinetic characterization of some bio dyes oil-in-water emulsions

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Emulsion stability is ensured by the zeta potential which measures the surface charge of droplets. Thus, the change of the zeta potential constitutes important information about the conditions of the interface which determines the stability of the emulsion. In the last years, emphasis has been on for more and more on edible/bio dye (derived from various sources: plants, insects and microorganisms) which offers several advantages. This study has shown that stable vegetable oil-in-water emulsions with bio dyes added to the aqueous phases (effective diameter 198.13 nm) can be prepared using a simple method that utilizes standard preparation procedures (homogenization and ultrasonication). The polydispersity value (dimensionless unit) was 0.196, which shows that the system is of nearly narrow distribution. These emulsions were relatively stable to droplet aggregation and creaming at 100 and 150 mM NaCl. However, the emulsions became more aggregated at higher ionic strength (200 mM NaCl). The experimental data obtained for zeta potential value of the bio dyes emulsions indicates that negative electrokinetic potential varies as follows: from 28.86 mV (pH = 5) to 46.74 mV (pH = 7). When the electrokinetic potential is low (less than 25 mV, absolute value), the attractive forces exceed the repulsive forces, and the particles come together leading to flocculation.

Keywords: bio dyes oil-in-water emulsions, size analysis, electrokinetic potential.

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The evaluation of serum electrolytes calcium, ionic calcium, magnesium and hemoglobin in Sulina’s patients, Danube Delta, Romania

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According to literature data, the normal values of biochemical parameters in blood vary by sex, age, geographical region and type of diet. The aim of this study was to analyze the benefits of a fish-based diet among the population of Sulina Town, in the Danube Delta. The batch of patients underwent a set of biochemical tests in the RoutineMed Laboratory of Sulina. The novelty of the research is represented by the geographic area covered, as the Danube Delta had no medical analysis laboratory until 2010, when RoutineMed Laboratory was opened in Sulina. Blood samples were collected from 260 patients (of 3663 residents) for the evaluation of the serum electrolytes: total calcium, ionic calcium, magnesium and hemoglobin. Both women and men were involved in the research and patients were grouped into age ranges: 20-40 years, 40-60 years, > 60 years. The study included 260 patients, of which 90 men (34.6%) and 170 women (65.4%), who declared they eat fish or fish-based products at least once a week. The values obtained were statistically analyzed using the SPSS v. 20 software and then compared to the ranges considered normal for these parameters. The results obtained showed that patients with a fish-based diet seem to be healthier than those with a diet in which fish meat is scarce, as their blood biochemical parameters values are closer to normal, which leads to the conclusion that including fish and fish products in people’s regular diet is beneficial.

Immunobiosensors based nano-carbons for detection of carbamate pesticides in horticultural products

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Pesticides play a major role in improving agricultural production through control of pest populations and plant diseases. Despite their merits, pesticides are considered to be some of the most dangerous environmental contaminants because of their ability to accumulate and their long-term effects on living organisms. The concern about the presence of pesticide residues in water, soil and food has prompted the search for alternative methods able to detect low levels of these compounds in a simple way. In this attempt, biosensors offer great advantages over conventional analytical techniques. In this work has been synthesized several carbon nanoparticles type *carbon xerogels and graphene oxide dispersions* for development of an immunosensor designed for some pesticide detection. Because electrical conductivity and high surface area provided by carbon nanoparticles make them viable as materials for bioelectroanalytical devices, surface area measurements and electrical conductivity characterization on obtained carbon nanoparticles has been done. Based on common use of porous nanostructures in biosensors for increase the quantity and activity of the immobilized biomolecules, parallel preliminary coupling experiments with antibodies has been initiated.

Ellipsometric characterization of thin surface layers for biosensor applications

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Characterization of surface layers for biosensor applications is of great importance to design stable functional coatings on biosensor transducer surfaces. Spectroscopic ellipsometry is a suitable technique to measure the refractive index and thickness of surface layers even at the nanometer scales, as well as to determine additional structural parameters (e.g. lateral homogeneity). In this work, gold layers on glass supports and carboxymethyl dextran (CMD) layers on optical waveguide lightmode spectroscopic (OWLS) sensor chips were characterized by ellipsometry using the developed optical models. Gold electrodes are widely used in electrochemical biosensors, its surface must be suitably prepared for further functionalization (e.g. protein deposition). The gold layers on the measured model samples were prepared by electron beam - physical vapor deposition (EB-PVD) on the glass supports, and then various cleaning methods were tested and discussed. The carbohydrate polymer dextran is proposed as a coating material for biosensor surfaces, primarily due to its high chemical modifiability, non-specific binding repellent ability and biocompatibility. The covalently attached CMD coatings (up to 100 nm) were prepared on the sensor chips using spin coating technique and further crosslinking process. Surface elemental compositions were determined by x-ray photoelectron spectroscopic (XPS) measurements.

Exploring the binding affinity between bovine β -lactoglobulin and β -carotene by using fluorescence spectroscopy and molecular modelling techniques

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β -Lactoglobulin (β -LG) can bind various hydrophobic compounds and drugs such as fatty acids, lipids, aromatic compounds, vitamins and polyamines. β -Carotenes (BC) are naturally occurring and widely used as a colorant in foods and beverages. However, the utilization of BC as a functional food in the food industry is currently limited because of its poor water solubility, high chemical instability, and low *in vivo* bioavailability. Encapsulation of BC can be used to improve the aqueous solubility, physicochemical stability, and bioavailability. The aim of the present study was to deepen understanding of thermal treatment effects on the β -LG-BC complex, in relation with protein structural changes as followed mainly by fluorescence spectroscopy and molecular modelling.

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Thermal stability of the complex formed by bovine alpha-lactalbumin and carotenoids from sea buckthorn investigated by molecular modelling techniques

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Sea buckthorn has gained importance as a versatile nutraceutical, due to its high nutritive value in terms of carotenoids. The SB berries contain high levels of various nutrients like vitamin C, flavonoid and oil soluble bioactive compounds such as tocopherols, tocotrienols, carotenoids, plant sterols, and triacylglycerols that increased the interest in its use as a functional ingredient. α -lactalbumin (α -LA) is the second most abundant whey protein and can be used to encapsulate different biologically active compounds. In this study, the thermal stability of the complex formed between α -LA and carotenoids from sea buckthorn were investigated by means of molecular modelling techniques.

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Contributions to the study on emulsions with walnut oil

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In this work has been studied the colloidal systems made with walnut oil. As surfactants were used so one hydrophilic (SDS) and one hydrophobic (Span 80). It was varied composition in the two phases of the emulsion and the surfactant concentration. Was studied the emulsions type obtained, as well as their stability. It has been found that emulsions prepared with SDS are simple direct emulsions, while the emulsions made with Span 80 are inverse emulsions double. Emulsions with SDS are more stable than emulsions with Span 80; phase separation time varies between one hour and several days – it was recorded a stable emulsion over a month. Emulsions with Span 80 are less stable; they are destroyed in minutes, but complete separation of phases takes place in a longer period. Span 80 emulsions with walnuts oil are more stable than those containing other food oils. This is due to the high viscosity of the walnuts oil.

SECTION 4

Electrochemistry. Corrosion. Ionic liquids.

KEYNOTES

Electrochemically triggered insulin release from graphene-based matrices

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Diabetes is a chronic disease characterized by an insufficient insulin plasma level to meet the organism demand. The actual treatment of type 1 diabetes is invasive and requires daily injections to regulate the glucose levels. The design of new non-invasive insulin delivery devices implying various (nano)systems and exogenous stimuli such as electrochemical, photothermal, pH and temperature triggered release were investigated. Our group approached the first-three methods using graphene-based systems. Electrochemical-stimulated insulin release from reduced graphene oxide (rGO) based-electrodes is particularly appealing. The electrochemical triggered insulin release proved to be potential dependent. Insulin concentrations of 7 μM were released in physiological media upon application of a potential pulse of -0.8V vs. Ag/AgCl for 30 min [1]. The quantity released is two orders of magnitude higher than the amount needed to decrease the diabetic blood glucose concentration to normal levels. The Western blotting analysis of electrochemically released insulin on hepatocyte cells evidenced that the biological activity of the released insulin is maintained [1].

[1] Teodorescu et al., *Chem. Commun.*, 51, 2015, 14167.

Computational investigation of some aliphatic amine inhibitors for silver corrosion

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Corrosion can be described as the undesirable reaction of a metal or alloy with the aggressive environment. Corrosion inhibition consists of the addition of chemicals known as corrosion inhibitors, which minimize the extent of corrosion. Practically all metallic materials are susceptible to corrosion under biased conditions in humid service environments, especially if aggressive ions are present. Silver corrodes easily in industrial environments containing such aggressive ions or in outdoor applications due to the humidity. Amines and their derivatives are well known as corrosion inhibitors and can effectively protect various metals from corrosion. The present study, prompted by the successful application of density functional theory (DFT) calculations in corrosion inhibitor research, is offered as a further contribution to gain a better understanding of the inhibition effect of four aliphatic amines, i.e., methylamine, ethylamine, n-propylamine, and n-butylamine (Fig. 1) for silver corrosion in nitric acid media, whose underlying mechanism is still far from explicit.

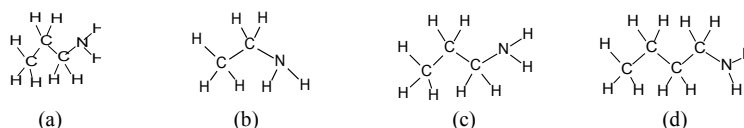


Fig. 1. Molecular structure of (a) methylamine, (b) ethylamine, (c) n-propylamine, and (d) n-butylamine.

SECTION 4

Electrochemistry. Corrosion. Ionic liquids.

POSTERS

Sn binary alloy coatings involving deep eutectic solvents as nanostructured anodes for Li/Mg ion batteries

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The paper presents some experimental results regarding the electrodeposition and physical characterization of Sn-Ni and Sn-Co alloy coatings involving choline chloride based eutectic mixtures, known also as “deep eutectic solvents”(DES). The electrochemical charge/discharge profile of nanoscaled Sn– Ni and Sn-Co alloy film electrodes were performed in choline chloride-urea eutectic mixtures containing 0.5-1 M MgCl₂. The obtained results suggested that the nanostructured Sn binary alloy coatings having a porous morphology allow Li/Mg intercalation/deintercalation and have higher capacity as compared to CoSb nanowires.

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Electrochemical Ag nanostructures involving deep eutectic solvents

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The paper presents some experimental results regarding the electrochemical synthesis of Ag based nanostructures (thin films and metallic nanoparticles) involving choline chloride based eutectic mixtures containing Ag(I) species., known also as “deep eutectic solvents”(DES). Some aspects regarding synthesis of different types of Ag based DES and physical characterization of the formed ionic liquid are also discussed.

Nanocrystalline pure Ag thin layers of a good quality and adhesion to the Cu substrate have been obtained.

Metallic Ag nanoparticles of 60-200 nm diameters have been also successfully synthesized in choline chloride-glycerol eutectic mixtures under reversed polarization conditions.

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Inhibition effect some nonionic surfactants of carbon steel in various aggressive mediaFlorina Branzoi¹, V. Branzoi², C. Pacuretu¹, I. Harabor² and A. Stanca³¹Institute of Physical Chemistry, 202 Splaiul Independenței, Bucharest, Romania, E-mail: fbrinzoi@chimfiz.icf.ro²University Politehnica of Bucharest, 132 Calea Griviței, Bucharest, Romania³Energy Research and Modernizing Institute, Bd. Energeticienilor no. 8, Bucharest, Romania

The inhibitory effect of some nonionic surfactants on the corrosion behavior of carbon steel type OL 37 in 1M H₂SO₄ and 0.5M HCl was studied by potentiodynamic polarization, electrochemical impedance spectroscopy, Fourier transform infrared spectroscopy and metallurgical microscopy techniques. In the present study, four types of organic inhibitors Span 80, Tween 80, Span60 and Tween 60 were investigated. The effect of inhibitor concentration on the corrosion rate, surface coverage and inhibition efficiency is investigated. Results show that these organic inhibitors exert a strong inhibiting effect on carbon steel corrosion and acts as a mix-type inhibitor. The inhibition efficiency of organic inhibitors may be due to either the adsorption of inhibitor molecules building a protective film or the formation of an insoluble complex of the inhibitor adsorption obeys the Langmuir model. The characterization using FT-IR demonstrates the adsorption of inhibitors and the formation of corrosion products on the electrode surface. The EIS measurements have confirmed this protection and pointed out the formation of adsorption layers on the electrode surface. The metallographic micrographies made before and after the potentiodynamic polarizations pointed out the evolution of the corrosion process. The addition of the organic inhibitors led in all the cases to inhibition of the corrosion rate. The thermodynamic parameters of adsorption enthalpy (ΔH^0), adsorption free energy (ΔG^0) and adsorption entropy (ΔS^0) were calculated. The inhibition process was attributed to the formation of the adsorbed film on the metal surface and blocking the active sites that protects the metal against corrosive agents.

**Electrochemical synthesis and characterization
on new polymer composite for OLC 45 corrosion protection**Florina Branzoi^{1*}, Viorel Branzoi², Cataliana Pacuretu¹ and Zoia Pahom²¹Institute of Physical Chemistry "Ilie Murgulescu"

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In this study, galvanostatic and potentiostatic electrodeposition mode was used for the synthesis of new composite (PPY-AOT/PNEA) coatings onto carbon steel of type OLC 45 for corrosion protection in 0.5MH₂SO₄ medium.

Monomer (N, ethylaniline) (NEA), pyrrole (PY) and anionic surfactant-AOT coatings have been electropolymerization on carbon steel by galvanostatic and potentiostatic synthesis techniques from aqueous solutions 0.1 M N, ethylaniline, 0.1M pyrrole, 0.01 M dioctyl sulfosuccinate sodium (AOT) and 0.3 M oxalic acid. In order to include dioctyl sulfosuccinate ions as dopant in the polypyrrole, AOT was also added to the polymerization solution of polypyrrole. The using of large anions increases the corrosion protection of the PPY film by preventing the penetration of aggressive ions. Characterization of new polymer composite coatings was carried out by cyclic voltammetry (CV), Fourier transform infrared (FT-IR) spectroscopy and scanning electron microscopy (SEM) techniques. Corrosion behaviour of PNEA-AOT/PPY coated carbon steel of type OLC 45 was investigated by potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) techniques in 0.5M H₂SO₄ solutions. The results of the corrosion tests showed that PNEA/PPY-AOT coatings ensure good corrosion protection of carbon steel in aggressive media.

Corrosion of some steels and aluminium alloys in the foam concentrate used as fire-extinguishing medium

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Corrosion of steel containers and aluminium nozzles in contact with firefighting foam liquids used to effectively extinguish fires has been studied. In general, in the fire engineering the fire fighting foam is made up of three ingredients - foam concentrate, water and air. The liquid concentrate is supplied from the manufacturer and when mixed with water in the correct proportion forms stable foam mass of small air-filled bubbles. The firefighting concentrate existing in the vessels from fire trucks is, however, corrosive and can make holes in the steel walls that are expensive to weld. Also, the nozzles made from aluminium alloys are destroyed due to corrosivity of foams during repeated usage. The FOAMTEC concentrates or other types are manufactured from synthetic foaming agents (hydrocarbon surfactants), solvents, fluoro chemical surfactants, small amounts of salts and foam stabilizers.

Values of corrosion current density, corrosion potential and polarization resistance were determined experimentally by using two electrochemical techniques: potentiodynamic polarization curves and electrochemical impedance spectroscopy. Also, some gravimetric measurements were performed in order to determine corrosion rate. SEM images allowed us to characterize the corrosion products.

Characterization of a new Ti-Zr-Nb alloy for implant applications

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A novel ternary Ti-15Zr-10Nb alloy with original properties and very good corrosion resistance for long-term in physiological solutions simulating the severe functional conditions of an implant was studied. Optical, XRD and SEM observations revealed $\alpha + \beta$ biphasic Widmanstätten microstructure with characteristic interleaving lamellae of $\alpha + \beta$ phases and good compositional homogeneity. The alloy has a Young's modulus of 64 GPa and very suitable mechanical properties for a good implant material. The alloy native passive film has a thickness of 5.5 ± 0.5 nm and contains protective TiO_2 , ZrO_2 and Nb_2O_5 oxides (XPS results). The cyclic voltammetry indicated a nobler electrochemical behavior of the alloy in comparison with Ti due to the beneficial influence of the alloying elements, which participate with their oxides to the compactness, thickening, reinforcement of the native passive film (XPS analysis). Alloy corrosion parameters had significantly better values than those of Ti, associated with more resistant, thicker, passive film. Nyquist and Bode diagrams showed a capacitive behavior, a passive film with higher insulating properties for alloy than those for Ti. The impedance results were modeled with an electric equivalent circuit containing two time constants: for inner, barrier, high protective layer and for porous, slightly inferior protective layer. The open circuit potentials ennobled in time, denoting the thickening of the passive film. BES-SEM micrographs confirmed the new depositions on the alloy surface consisting of carbonated calcium phosphate (EDS spectra). The open circuit potential gradients had very low values, which can not initiate galvanic cells for 1500 immersion hours in acid, neutral and alkaline Ringer's solutions.

The fractal analysis of self-assembled monolayers of L-cysteine on GaAs (100) electrodes

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Some L-cysteine modified p- and n-GaAs(100) electrodes have been investigated by fractal analysis of atomic force micrographs (AFM).

The "box-counting" method, the information method, the correlation function method and the variable length scale method were used to describe the fractal behaviour of the surfaces. Fractal dimensions were computed and, also, the fractal curves were analysed to determine the characteristic "fractal print" of each image.

To compute the "box-counting" fractal dimension and the information fractal dimension, the grey level images were converted into black-and-white images considering a grey level threshold. The dependence of the "box-counting" dimension and of the information dimension on the threshold grey level was also depicted.

Fractal analysis shows that L-cysteine monolayer changes the self-similarity behaviour of both substrates. The L-cysteine covered p-doped substrates depict only one fractal dimension with remarkable long-range self-similarity, meanwhile the L-cysteine covered n-doped samples reveal two different fractal dimensions.

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Peroxynitrite sensor based on a modified screen printed Carbon electrode

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A peroxynitrite sensor based on screen printed electrode modified with an electropolymerized film is reported. The film resulted from the electropolymerization of 2,6-dihydroxynaphthalene (2,6-DHN) was used showed an electrocatalytic effect on the peroxynitrite oxidation. The modified sensor allows detection of peroxynitrite at a much lower potential (+0.1V) comparing with the unmodified one (+0.9V). The analytical performances of peroxynitrite sensor were optimized by studying the influence of the electropolymerization conditions: electrochemical technique used (cycling voltammetry, potentiostatic), 2,6-DHN concentration, scanning potential range, number of scans, scan rate etc. The analytical features of the optimized sensor were evaluated regarding the linear concentration range of peroxynitrite, LOD, sensitivity, intra-day and inter-days reproducibility, stability of the response in operational and in storage conditions, potential interferences, etc. The developed peroxynitrite sensor showed excellent properties for a screen printed electrode based sensor (LOD = 10 μ M, concentration range 10 – 350 μ M, RSD intra-day and inter-days < 3,5%).

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Corrosion resistance of a new dental CoCrNbMoZr alloy in comparison with commercial one

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The microstructure, mechanical and anticorrosive properties of the new CoCrNbMoZr alloy were studied in comparison with those of the commercial CoCrMo, Heraenium CE alloy. XRD and SEM techniques were used to evince the microstructure, respectively the morphology of the two alloys. Electrochemical linear and potentiodynamic polarization and electrochemical impedance spectroscopy methods showed the electrochemical and corrosion behavior of the alloys in artificial Carter-Brugirard saliva of different composition (doped with NaF, pH = 8.21 and undoped) and pH values (3.83; 7.84; 9.11) simulating the various functional conditions from the oral cavity. The new CoCrNbMoZr alloy showed self-passivation, more favorable values of the corrosion, passivation and transpassive potentials and tendency to passivation than those of the commercial Heraenium CE alloy and lower values of the passive current density; the values of the corrosion current densities and corrosion rates are lower and polarization resistances are higher comparing with those of the reference alloy. EIS spectra revealed for the new alloy a passive film, a compact, resistant layer formed especially by the chromium, cobalt, niobium and zirconium oxides. Taking into consideration the microstructural features, electrochemical behavior, corrosion resistance, mechanical characteristics, it results that the new CoCrNbMoZr alloy is recommended for dental applications.

The inhibiting effect of Tris (hydroxymethyl) aminomethane (TRIS) on the corrosion of metal iron

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The corrosion of metal iron, one of the most important materials, is an important problem that limits its use. During the last decades, there were realized countless studies having as a major purpose the control of the iron corrosion process.^[1] It was demonstrated that a large number of organic compounds which contain in their molecule atoms of nitrogen, oxygen and sulfur can decrease the rate of corrosion. The three atoms of N and one atom of O contained by tris (hydroxymethyl) aminomethane (TRIS) give it an important potential for inhibition of iron corrosion.

In this study has been investigated the corrosion of iron (purity 99.9%) in acid solution (pH 2.5) of TRIS (0-1 mM) at 27°C by electrochemical (Potentiodynamic Polarization and Cyclic Voltammetry) and aqueous batch experiments.

The analysis of the polarization curves using Tafel method indicates a decrease in corrosion current density (i_{corr}) from 87 $\mu\text{A}/\text{cm}^2$ (0 mM) to 33 $\mu\text{A}/\text{cm}^2$ (1 mM). The inhibition efficiency (IE), calculated using the formula $IE = (1 - i_{\text{corr}}/i_{\text{corr}}^0) \cdot 100$, demonstrates that TRIS inhibits the iron corrosion process. Its inhibition efficiency increases with increasing the concentration of organic compound.

[1] E.M. Sherif, Mater. Chem. Phys. 129 (2011) 961-967.

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Sonogel-carbon based biosensors prepared using sinusoidal voltages method

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Biosensors are very useful tools to determine analytes in complex matrixes. Conducting Polymers (CPs), such as PEDOT, including enzyme (Tyrosinase, Ty) can be used to successfully modify the physicochemical properties of the transducer material. The new improvements are based on the simultaneous enzyme and PEDOT electrochemical deposition using sinusoidal voltages. In this work, CPs are deposited on the surface of the Sonogel-Carbon electrodes (this material has excellent properties like transducer material), using several electrochemical procedures. Besides, PEDOT-Ty biocomposite materials are also deposited on the surface of these electrodes. Analytes of interest such as, dopamine, hydroquinone, and ascorbic acid have been determined. The analytical performances of these biosensors have been also assessed. Finally, the target analytes have been successfully quantified in biological and environmental real samples.

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Electrochemical study of the lanthanides coordination with pyridine heterocycles

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The synthesis of new lanthanide complexes relates to their interesting properties. They were synthesized by using quaternary pyridinium salts derived from 4,4'-bipyridinium and 1,2-bis-(4-pyridinium)ethane, lanthanum (III) and neodymium (III) sulfate in methanol and studied by cyclic voltametry (CV-Bio-logic SP 50) to predict their behaviour in medical applications. Cyclic voltammograms registered show changes in the redox potential of the complexes compared to the free N-heterocyclic ligands and this behaviour dependent on the pH, the potential and on the scan rates applied. The voltammograms in aprotic solution (DMSO) indicates enhanced electronic transfer processes of one/two electrons compared to the aqueous or alcoholic medium. Ethylene group from the N,N'-bis (p-bromophenacyl)-1,2-bis(4-pyridyl)-ethane dibromide induces changes in the electrochemical performance in comparison with the ligand N,N'-bis(p-bromophenacyl)-4,4'-bipyridinium dibromide and determines preferential arrangements in complexes. An influence from La³⁺ or Nd³⁺ ions is also observed in complexes structure. Ligands conductivity is different in the aprotic compared with the aqueous or alcoholic medium, indicating differences of the protonated/deprotonated form of the free ligands and also complexes. The electrochemical properties indicate and recommend novelty compounds in some biomedical applications.

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Electrochemical biosensors based on microelectrode arrays for phenol electroanalysis

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The aim of this work is the development of an electrochemical microbiosensor based on microelectrode arrays modified with poly(3,4-ethylenedioxythiophene) conducting polymer and tyrosinase (Tyr) for phenol determination. The novelty of this work lies on the use of sinusoidal voltages (SV) method on fixed frequency ranges and values in order to highlight the improvement in the analytical performance of the proposed biosensor. The enzymatic activity of Tyr in homogeneous solution was assessed by using UV-Vis spectrometry and L-Dopa as substrate, and compared to that of the immobilized Tyr determined from electrochemical measurements. The optimization of the biosensor's preparation was achieved using the electrochemical quartz crystal microbalance (EQCM). Both the frequency change of crystal resonator, the applied SV signal and the current response of the systems were recorded simultaneously. The influence of the d.c. potential value for electrochemical polymerization of the monomer, as well as the frequency and amplitude of the SV signal were optimized. The analytical performance of the proposed biosensor, in terms of limit of detection, linear response range, response time, sensitivity, repeatability and reproducibility, was also assessed.

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Multianalyte detection of dopamine and hydroquinone at electrochemical microbiosensors

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The present work is focused on the simultaneous determination of DA and hydroquinone (HQ) at gold microelectrode arrays modified by biocomposite materials consisting of poly(3,4-ethylenedioxythiophene) conducting polymer and tyrosinase (Tyr). The microbiosensors are prepared by using a sinusoidal voltages (SV) preparation procedure consisting in the application of a sinusoidal voltage over a suitable d.c. potential. The improvements with respect to our previous works lie on the use of SV of fixed frequency and d.c. potential values where no electrochemical polymerization process takes place. This allows for the evaluation of the contribution of SV component only to the development of the electrochemical biosensors. Several electrochemical parameters such as the fixed frequency value, the amplitude of SV, and d.c. potential value were optimized. A multianalyte detection protocol for DA and HQ determination from a sample mixture by using bipotentiostatic measurements has been developed. The biosensor prepared at SV of 50 mHz frequency displayed the best analytical performance for two-analyte detection, i.e. the limit of detection for DA in the presence of 300 μM HQ was of 0.66 μM , and the recovery for DA was close to 100.2 %. This biosensor was successfully applied in DA determination in pharmaceutical formulations.

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Interactional effect of the titanium substrate on photo-electrochemical behavior of TiO₂ nanotubes

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The synthesis and characterization of thin film based on ordered array of TiO₂ nanotubes supported on Ti metallic substrate are investigated. By using the anodic oxidation procedure (based on the electrochemical etching of titanium foils in electrolytes containing fluorides) it is thus possible to develop novel type of catalytic materials and electrodes for sustainable energy applications. The morphology and surface characteristics of TiO₂ nanotubes were investigated using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX) and Raman spectroscopy, respectively. The nanotubular TiO₂ layers consist of individual tubes of about 90-110 nm diameters. Electrochemical characterization of TiO₂ nanotubes was performed by EIS measurements and the photo-induced effect was also investigated. Evaluation of electrical properties was achieved before and after UV exposure to check the presence of long lasting effects due to UV illumination. The results confirmed that photocurrent depends on the interaction with the metallic Ti substrate and the electrical resistance at the interface, besides to other aspects such as TiO₂ NT thin film thickness and morphology. **Acknowledgements:** This work was supported by a grant from to the Romanian National Authority for Scientific Research, CNCS-UEFISCDI Project number PN-II-ID-PCE-2011-3-0272 (PN II IDEI 41/5.10.2011)

Electrochemical monitoring of oxidative stress-related biomarkers

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The oxidative stress is determined by the imbalance between oxidants and antioxidants in the body and might be involved in different diseases such as neurological disorders, cancers, liver damages etc. The monitoring of corresponding biomarkers is very important both for diagnostic purpose and for the assessment of diseases progresses as well. In this work a simple, rapid and selective electroanalytical method for the assessment of uric acid (UA), ascorbic acid (AA) and lipoic acid (LA) was developed and subsequently applied to a human serum sample. The differential pulse voltammetry (DPV) was employed to study the electrochemical oxidation of AA, UA and LA. The voltammetric curves recorded at a platinum electrode when biomolecules of concentrations close to physiological levels are simultaneously present in aqueous saline buffered solutions of pH 4.5 have showed oxidation peaks occurring at 340 mV for AA, 540 mV for UA and 710 mV for LA. The well separated oxidation peaks together with good electroanalytical performances such linear response within the range 10-800 μM LA and detection limit of 13.15 μM LA allowed the application of the developed method to electrochemical determination of LA in real samples. Accordingly, 20 μL of human serum from a patient with stroke were diluted in acetate buffered solution (pH 4.5) and subjected to voltammetric measurements after spiking with different concentrations of LA. The concentration of the LA in serum sample determined from voltammetric measurements was of 15 μM.

Evaluation performance $\text{La}_{0.5}\text{Sr}_{0.5}\text{Co}_{0.8}\text{Fe}_{0.2}\text{O}_{3-\delta}$ (LSCF) and $\text{Nd}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.8}\text{Cu}_{0.2}\text{O}_{3-\delta}$ (NSCC) thin films cathodes for IT-SOFC

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In order to evaluate the performance of the $\text{La}_{0.5}\text{Sr}_{0.5}\text{Co}_{0.8}\text{Fe}_{0.2}\text{O}_{3-\delta}$ (LSCF) and $\text{Nd}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.8}\text{Cu}_{0.2}\text{O}_{3-\delta}$ (NSCC) cathodes for IT-SOFCs application, symmetrical cells based on thin films cathodes have been developed. The LSCF and NSCC perovskites thin films were deposited on by pulsed laser deposition technique on the both sides of commercial YSZ pellets heated at 1200°C. The process was conducted in oxygen atmosphere (1.3×10^{-1} mbar) by using an Ar*F excimer laser at 193 nm, at a fluence of 5 J/cm² and a frequency repetition rate of 40 Hz. The structural properties were investigated by XRD, the morphology and topography were assessed by SEM and AFM. The surface chemistry analysis was performed by XPS and the performance of the symmetrical cells was evaluated by electrochemical impedance spectroscopy. Measurements were performed in air, in the temperature range 500-800°C. The sample NSCC exhibited the lowest area specific resistance at temperatures lower than 700°C.

Acknowledgements

The financial support from UEFISCDI in the framework of research project PN-II-PT-PCCA-2011-3.1-1423 (no 26/2012) is gratefully acknowledged.

Study of the crystal structure of the surface, the magnetic properties and corrosion resistance of the modified steel for special applications

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The corrosion action processes in different aqueous and ionic liquids media on the surface morphology, crystal structure and magnetic characteristics of some modified special steels was studied. Corrosion studies were carried out on OL44, OL52 and S4571 steels in different ionic liquids and corrosion parameters were calculated. The crystal structure was studied by using an X-ray diffraction method and the specific magnetization was investigated by ponderomotive method. The elemental composition, elements distribution maps, coatings surface images are obtained using X-ray microanalyzer Hitachi S5500. The micrographic images of the studied samples before and after corrosion were obtained with a metallurgical microscope (USA) with a digital camera for images acquisition

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**The oxidative dissolution of pyrite (FeS₂) in the presence of sodium carbonate.
The use of carbon paste electrodes (CPE)**

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Pyrite is the most abundant terrestrial metal sulfide. It is usually associated with other metal sulfides, coals, and uranium ores. The aqueous oxidation of pyrite is a reaction involved in various natural and industrial processes like acid mine drainage (AMD) formation, metal extraction and ore processing.^[1]

This study follows to investigate the oxidative dissolution of pyrite in the presence of sodium carbonate using electrochemical methods. Electrochemical measurements were performed with a carbon paste electrode (CPE) covered with FeS₂ powder and immersed in 0.01 M Na₂CO₃ solution (pH 10.5), at 25°C. The errors associated to the oxidation current density (i_{ox}) decrease from 98% to 13% when the pyrite particles used for CPE building were ultrasonicated for 20 min. It is worth to note that the determination of the oxidation potential (E_{ox}) is less affected by the ultrasonic pretreatment of pyrite particles.

[1] C.A. Constantin, P. Chirita, J. Appl. Electrochem. 43 (2013) 659-666.

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**Characterization of a biomimetic coating
applied on surface of new ternary Ti-Ta-Zr alloy**

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The surface of the new ternary Ti-15Ta-5Zr alloy was functionalized with bovine serum albumin (BSA) deposited by chemical method adapted to the composition of the alloy and its passive film. The BSA deposition was proved by atomic force microscopy (AFM), scanning electron microscopy (SEM) and Raman micro-spectroscopy techniques; also, its electrochemical behavior and corrosion resistance in physiological Ringer solution of different pH values were performed by cyclic potentiodynamic and linear polarization and electrochemical impedance spectroscopy (EIS). The BSA coating consists from quasi-spherical aggregates (AFM) with high roughness which can promote the osteoblast cell development. SEM micrographs revealed a thick deposition with some porosity. EDX spectrum identified C and N elements from BSA and Ca and P from the deposition solution which can stimulate the bone formation. Raman spectra showed the similar composition of BSA powder and BSA deposited on the Ti-15Ta-5Zr alloy surface. Electrochemical parameters have more favorable values for the BSA coated alloy comparing with the bare alloy proving nobler electrochemical behavior of BSA coated alloy. Corrosion parameters have superior values of about 3-10 times than those of the bare alloy. The impedance results were fitted with two time constants electric equivalent circuit for the bare alloy and with three time constants for the coated alloy. The impedance results evinced the dual character of the surface of the BSA covered alloy: corrosion resistance and bioactivity that stimulates the growth of the bone cells, favoring the alloy osteointegration.

**The application of deep eutectic solvent ionic liquids
for electrocatalytic dissolution and recovery of metals from WEEE**

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This paper demonstrates that deep eutectic solvent (DES) ionic liquids provide the processing of waste electric and electronic equipments (WEEE) since they can be used to selectively dissolve and recover copper, tin, lead, gold and silver. Ionic liquids are anhydrous salts that are liquid at low temperature. They are powerful solvents and electrolytes with potential for high selectivity in both dissolution and recovery. Deep eutectic solvents are a form of ionic liquid that are mixtures of salts such as choline chloride (ChCl) with hydrogen-bond donors such as urea or ethylene glycol. DESs are environmentally benign, yet chemically stable and, furthermore, the components are already produced in large quantities at comparable costs to conventional reagents. The dissolution and selective recovery of Cu, Sn, Pb, Au and Ag from WEEE necessitates redox chemistry. Here, deep eutectic solvents are used to simplify the speciation of solutes and to allow redox potentials to be modified, compared to standard aqueous values. The redox catalyst used is iodine, as it demonstrates high solubility, fast electron transfer and the ability to oxidise most elements and the efficacy of this electrocatalytic method was demonstrated using two samples: multicomponent alloy and mud obtained by pyrometallurgical technology from WEEE. Finally the metals electrodeposition mechanism was studied by cyclic voltammetry and a two steps mechanism was found for Cu while an one step mechanism for Pb, Sn, Ag, Au.

**Control of the electronic properties of p-GaAs(111)B surface
by using aliphatic and aromatic dithiols**

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X-ray photoelectron spectroscopy and electrochemical investigations attest that the functionalization of p-GaAs(111)B surface with dithiols allows the control of chemical and electronic properties of the semiconductor. XPS data point out that the spontaneously self-assembled monolayers on p-GaAs(111)B from aromatic and aliphatic dithiol solutions provides a good protection against oxidation in air of the semiconductor surface, which is better for the aliphatic thiolate. These results are in good agreement with the information derived from EIS measurements which indicates a diminution of the population of surface/interface states of semiconductor after its chemical modification with dithiols, more pronounced in case of the aliphatic thiolate. It appears that aliphatic dithiol is more appropriate for improving chemical and electronic properties of the p-GaAs(111)B substrate for further biosensors and electronic applications. One may conclude that chemically modified p-GaAs(111)B substrate with dithiols may represent options for developing new electronic devices or biosensors.

Electrochemical synthesis and characterization of CoSb nanowires used as anode in batteries with ionic liquid

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Co-Sb nanowires were obtained with different amount of Sb. Electrochemical deposition method open the way for new technologies and nanomaterials with unique properties achieving. The Co-Sb nanowires have an approximate length is between 3 and 6 microns and a different diameter. These materials may be used as a nanostructured anode in batteries, to improve their properties.

The surface morphology, the structural and elemental analysis of nanowires formed on the working electrode was studied using scanning electron microscopy.

Charging-discharging cycles were performed in two types of ionic liquids based on choline chloride were tested. Cyclic voltammetry curves show that the electrochemical ion insertion process is carried out very well. The dissolution of large quantities of Mg^{2+} ions in ionic liquid choline chloride urea cycle reveal a greater amount of charge compared to the same ionic liquid in which dissolved 0.5M $MgCl_2$. To test the CoSb nanowires electrochemically obtained in order to use them as an anode in batteries, electrochemical impedance spectroscopy tests were performed.

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Nanostructured anode for batteries with ionic liquid based choline chloride

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TiO_2 nanotubes growth on Ti samples (99.9% purity) with 1 mm thickness were used as substrate. Samples were grinded on SiC paper with different grits such as 500, 800, 1200, 2400 and 4000. The samples were then degreased in acetone and ethanol successively (5 min each) in an ultrasonic bath, followed by rinsing with deionized water. TiO_2 nanotubes were obtained by electrochemical anodizing using a two-electrode configuration with platinum as cathode and Ti substrate as anode. The used electrolytes were etilen glycol + 2%v/v H_2O + 0.5wt% NH_4F . The potential was swept from 0 V to 20 V with either 0.1 V/s or then the potential was kept constant at the desired anodizing potential. All electrochemical anodizing experiments were carried out at room temperature.

Two types of ionic liquids based on choline chloride, one mixed with urea and other with ethylene glycol were electrochemically characterized in terms of charge-discharge cycles. Best results confirmed the answer given by all test electrodes to be used as anode in choline chloride with urea. Mg^{3+} ionic insertion is done better and longer nanotubes with average diameters (50-80 nm). Cyclic voltammetry cuves show that the electrochemical ion insertion process is carried out very well.

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Electrochemistry of photoswitching systems based on fluorescent azulenyl-substituted dithienylcyclopentenes

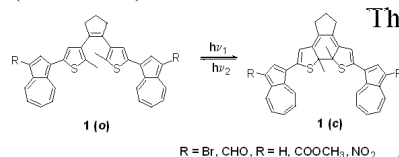
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Molecular switches that can reversibly change their properties upon excitation with light or other external stimuli have recently received considerable attention due to their potential applications for molecular electronic devices such as memories and switches.¹ Although the field of molecular switches is rapidly growing, the number of photochromic systems in which the photocyclisation reaction is achieved by irradiation with visible-light is very scarce.² We have recently shown that tailoring the thiophene rings of the dithienylcyclopentene photochromic system with azulene moieties (Scheme 1) resulted in a visible-light induced photocyclisation process.³



The electrochemical ring-closure electrochemical switching between the open and closed states of compounds **1** was examined by cyclic voltammetry. All studied compounds showed similar cyclic voltammogram profiles with oxidative ring-closure of the dithienylethene group above 1.70 V. The electrochemical mechanism was interpreted by corroborating the CV experiments with spectroelectrochemistry and DFT calculation as being a two-electron oxidation of the open form **1(o)**²⁺ to **1(c)**²⁺.

¹M. Irie, Y. Yokoyama, T. Seki, *New Frontiers in Photochromism*; Springer, Japan, 2013.

²*Angew. Chem., Int. Ed.*, 2016, **55**, 1208. ³*RSC Adv.*, 2015, **5**, 63282.

Improvement of supported Platinum particles resistance to fouling by appropriate selection of the substrate

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Despite the tremendous amount of research work channeled so far towards finding active, noble metal-free, electrocatalytic materials, it appears that platinum still remains the main choice for high efficiency electrochemical oxidation of small organic molecules. For obvious economic reasons, more extensive implementation of platinum-based electrocatalysts requires minimization of the noble metal loading, while maintaining high activity. The most straightforward way to solve this problem is to deposit the active material as small particles on a stable, electrically conductive, support material, thus enhancing both the specific surface area of the electrocatalyst and its accessibility. A more complex issue rises from the fact that, during oxidation, reaction intermediates (e.g. CO) remain adsorbed on the Pt active sites, with deleterious effects on the long-term activity of the electrodes. To alleviate this drawback, the possibility of developing new electrocatalytic materials was investigated, based on a “bifunctional” approach. It was found that oxygenated species adsorbed at Pt particles (or at their substrate) in the vicinity of blocked Pt sites can act as oxygen donors and may facilitate further oxidation of adsorbed intermediates. This process regenerates, at least partially, active sites from the electrocatalyst surface contributing much in maintaining high activity over the projected lifetime of the electrodes. **Acknowledgements:** This work was supported by a grant from to the Romanian National Authority for Scientific Research, CNCS–UEFISCDI Project number PN-II-ID-PCE-2011-3-0272 (PN II IDEI 41/5.10.2011)

Role of Iridium oxide in the reactivation of Platinum nanoparticles electrodeposited at BDD powder

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Bare boron-doped diamond powder (BDDp) and BDDp modified by thermal iridium oxide deposition were used as substrates for platinum particles. Both Pt/BDDp and Pt/BDDp-IrO_x electrodes obtained by ink-paste method on glassy carbon surface exhibited voltammetric responses typical of platinum behaviour in acidic media. To assess the activity for methanol oxidation of the two types of electrodes, long-term polarization measurements were performed in a 0.1 M NaOH solution, containing methanol. Before and after prolonged electrolysis, electrochemical impedance spectroscopy (EIS) experiments were carried out at an applied potential close to the half peak value. Compared to Pt deposited on bare BDDp, a better activity of the Pt/BDDp-IrO_x system for methanol oxidation was evidenced by long time polarization. The results of chronoamperometric and impedance experiments indicated that, when deposited on the BDDp-IrO_x powder substrate, platinum particles are less susceptible to deactivation via CO poisoning during methanol oxidation.

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Electron Structure Effects in Boron Doped Diamond

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The features making the boron doped diamond suitable as electrode are investigated by computational experiments aiming to detect the local electron structure modifications induced in environment by a boron atom and the long range interaction between boron sites. The local B site can be characterized as a hole in a degenerate level, prone to distortions of Jahn-Teller type, as the corresponding potential energy surface mapping illustrates. The unpaired electron originating from the boron atom appears rather delocalized on the neighboring atoms, explaining the conducting behavior of the doped diamond. The strength of the interaction between boron sites is tested estimating by Broken Symmetry Density Functional calculations the exchange coupling constants in diradical systems with two B atoms, taken as large molecular fragments, cut from the lattice. We found a rather strong communication between the B atoms, up to distances in the range of ten angstroms, a fact also in line with the conducting functionalities.

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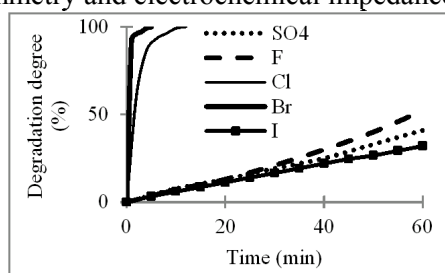
Electrochemical degradation of coloring food Brilliant Blue FCF from simulated wastewaters

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Coloring food additives include dyes such as azo-compounds with negative impact on human health and wastewaters characteristics.

The electrochemical degradation of E-133 coloring food dye (Brilliant Blue FCF) on platinum electrode has been studied by photo-assisted current constant electrolysis ($i = 50 \text{ mA}\cdot\text{cm}^{-2}$), cyclic voltammetry and electrochemical impedance spectroscopy.



Time variation of E-133 degradation degree (%) with time for electrolyzed solution $2 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$ E-133, $0.1 \text{ mol}\cdot\text{L}^{-1}$ NaX (X = SO₄, F, Cl, Br, I) on Pt electrode.

Experimental results showed that by changing the nature of the supporting electrolyte, the degree of degradation increases in the following order: $\text{I} < \text{SO}_4 < \text{F} < \text{Cl} < \text{Br}$.

The study of nystatin drug stability by electrochemical and thermal analyses

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The physico-chemical stability of Nystatin drug, used to treat Candida infections, has been studied by linear polarization, cyclic voltammetry and thermogravimetric analyses. Electrochemical degradation of nystatin by current constant electrolysis ($i = 50 \text{ mA}\cdot\text{cm}^{-2}$) of $5 \times 10^{-5} \text{ M}$ nystatin, 0.1 M NaCl solution on different electrodes (Pb, Ni, Cu, Pt) was analyzed by spectrophotometry method. The results indicate that the degradation degree (figure 1) of nystatin drug is strongly influenced by the nature of electrode material, reaching a maximum value of 100 % on Platinum electrode after 13 minutes of electrolysis.

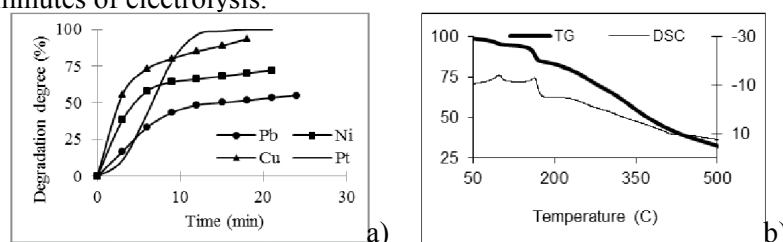


Figure 1. Time variation of degradation degree for $5 \times 10^{-5} \text{ M}$ nystatin, 0.1 M NaCl solution on different electrodes, a) and TG/DSC curves of nystatin, b)

Thermogravimetric curve (TG) indicates a gradual decomposition starting above $160 \text{ }^\circ\text{C}$. DSC (differential scanning calorimetry) curve indicates two associated endothermic effects at $90 \text{ }^\circ\text{C}$ and $160 \text{ }^\circ\text{C}$.

Passive film behavior of new quaternary Ti based alloy

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A new quaternary Ti-20Zr-5Ta-2Ag alloy with innovative composition and properties was elaborated to fulfill the necessities of corrosion resistance, biocompatibility and antibacterial protection; Zr and Ta, non-toxic alloying elements improve both mechanical, anticorrosive and biocompatibility properties and Ag induces antibacterial activity by a lent release of silver ions in the human electrolyte. The new Ti-20Zr-5Ta-2Ag alloy was characterized regarding its microstructure, its native passive film composition and thickness, its electrochemical behavior in Ringer solution of different pH values. The new alloy has a bi-phase, $\alpha + \beta$, acicular, homogeneous microstructure (SEM). Its native passive film (12 nm thicknesses) consists from protective TiO_2 , ZrO_2 , Ta_2O_5 oxides, Ti and Ta suboxides and metallic Ag (XPS data). The main electrochemical parameters of the new alloy are superior to Ti as result of the beneficial influence of Zr, Ta, and Ag alloying elements which reinforce its native passive film. EIS spectra in Ringer solutions displayed better values of impedances and phase angles proving a more insulate passive film than that on Ti surface. The main corrosion parameters for the new Ti-20Zr-5Ta-2Ag alloy are more favorable of about 25 – 38 times than those of Ti, confirming very resistant passive film. The new Ti-20Zr-5Ta-2Ag alloy releases into Ringer solution low quantities of Ti^{4+} , Zr^{4+} metallic ions. Ag^+ ions are released in low quantity conferring to this alloy antibacterial activity. All experimental results show that the new Ti-20Zr-5Ta-2Ag alloy fulfils the requirements for the biocompatibility, corrosion resistance and antibacterial protection.

SECTION 5

Advanced materials science

KEYNOTES

Coordination polymers based on cyanido complexes

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The design of coordination heterometallic networks is of high interest especially in molecular magnetism and crystal engineering, due to the potential applications of these compounds as molecular magnets, porous and catalytic materials, or multifunctional materials. The node and spacer approach, formulated by Robson in 1990, represents a powerful strategy to construct coordination polymers with various dimensionalities and network topologies. Following this strategy, we use as nodes mono- or bimetallic complexes and as spacers, metalloligands. Cyanido metalloligands are widely employed for building heterospin networks due to the ability of the cyanido bridges to efficiently mediate magnetic interactions between paramagnetic metal ions. For this communication, the focus will be on the 3d heteroleptic cyanido complexes, $[M^{III}L(CN)_4]^-$, which were successfully used in the synthesis of heterometallic coordination polymers (L = bidentate blocking ligand; $M^{III} = Fe, Cr$). The crystal structure and magnetic properties will be discussed.

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Mesoporous inorganic carriers for biologically active molecules

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Various studies are focused on the development of new drug delivery systems (DDS) based on clinically used active pharmaceutical ingredients (API) in order to improve their therapeutic characteristics: controlled delivery, minimization of side-effects, enhancement of dissolution rate of poorly water soluble drugs, targeting the ill tissue etc. A vehicle for a drug must be biocompatible and able to load the required amount of API, to preserve its therapeutic response and to release it gradually over time. Ordered mesoporous silica and aluminosilicates with different pores size and geometry can be employed as carriers for various drugs due to their high adsorption capacity. To tailor the interactions between the carrier and biologically active molecules, the surface properties of silica can be modified by binding different organic groups. A series of pristine and functionalized mesostructured silica and aluminosilicates, which belong to MCM-41, MCM-48 and SBA-15 classes, were synthesized, characterized and employed by our group as carriers for different antibiotics (amikacin, kanamycin, oxytetracycline) and cytostatic agents (irinotecan and aminogluthetimide). The *in vitro* cell viability results indicated that the studied mesoporous silica and aluminosilicate carriers did not induce significant cytotoxicity within different cell lines. For the prepared DDS the drug delivery profiles depend on the interactions between the drug molecules and mesoporous matrix. Similar or improved therapeutic effect was observed for DDS comparing with the drug alone.

Studies on the solubility enhancement of norfloxacin by encapsulation in pristine and functionalized mesoporous silica

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Mesoporous silica materials can be applied in various fields including matrices in drug delivery systems. In this study, norfloxacin, a very slightly soluble drug, which belongs to the quinolone antibacterial class, was used to prepare drug delivery systems based on mesoporous silica in order to assess the influence of textural properties and surface modification of the carriers on the drug release profiles. For this purpose, pristine and functionalized mesostructured silica materials with different pore size and geometry and surface modification with hydrophobic and hydrophilic groups were used. The drug adsorption into the mesopores of the mesostructured-silica carrier was performed through incipient wetness impregnation method. The mesostructured silica materials and norfloxacin-based composites were characterized by small-angle and wide-angle X-ray diffraction, N₂ adsorption/desorption isotherms, FT-IR spectroscopy and thermogravimetric analysis. The norfloxacin release profiles were performed *in vitro*, in simulated body fluid, pH=7.4, and showed an increased solubility of the drug.

High entropy oxides: a new class of functional materials

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Since the early 2000s, an intense research activity is devoted to the study of high-entropy alloys, which have very interesting properties for many applications. These alloys are obtained by entropy stabilization of single phases from complex mixtures of typically 5 metals. Recently, this concept has been extended to oxides and it has been shown that the entropy stabilisation of a solid solution from a mixture of MgO, NiO, CoO, CuO, and ZnO is possible. This structure is stabilized by the large configurational entropy arising from the site distribution of the five cations.

Following this study, we have shown that the compounds of this new class of oxides may be substituted or co-substituted, which leads to a considerable number of possible chemical compositions.

Furthermore, we studied the physical properties of some specific compounds which are extremely promising for applications such as colossal dielectric constant and super ionic conductivity. During this presentation, we will describe some new compositions belonging to this peculiar family and their outstanding transport properties.

Four different crystals and one synthesis: a case of supramolecular isomerism snapshotting a stepwise chirality transfer

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When identical components of a network (i.e. metal ions, organic molecules acting as ligands, solvent molecules) generate building-blocks which eventually assemble into different superstructures (i.e., discrete entities or 1D, 2D, or 3D networks), supramolecular isomers are afforded. Generally speaking, supramolecular isomerism originates from structural, conformational, catenane and/or optical subtle variations of the given set of readily available molecular moieties.

In our case, the latter factor plays the ultimate role: in the first isolated crystal, the *in situ* formed M- $\{\Delta\text{-Cu}(\lambda\text{-tmen})(\text{mipt})_2\}^{2-}$ and P- $\{\Lambda\text{-Cu}(\delta\text{-tmen})(\text{mipt})_2\}^{2-}$ helicoidal fragments (tmen = *N,N,N',N'*-tetramethyl-ethylenediamine, H₂mip = 5-methoxy-isophthalic acid) are alternately connected by supplementary copper(II) ions into a γ -shaped achiral homonuclear chain. Following a spontaneous resolution, two chiral crystals containing P- and M- $[\text{Cu}(\text{tmen})(\text{mitp})]$ single-stranded helicate, respectively, are separated from the reaction solution. The guest water molecules construct chiral columns based on incomplete adamantane eight member rings. The last achiral crystal consists in adjacent P- and M-chiral chains generated by $[(\text{tmen})\text{Cu}(\mu\text{-OH})\text{Cu}(\text{tmen})]^{3+}$ nodes and mip²⁻ spacers. Where relevant, spectroscopic, magnetic and/or thermal behaviour is analyzed.

New keys for the keywords of molecular magnetism. A chemist's perspective on the magnetic anisotropy.

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The magnetic anisotropy is a running paradigm of the nowadays molecular magnetism, stirring interest both from academic and application perspectives, its mastering leading to the understanding and prediction of the systems behaving as magnets at molecular and nano-scale levels. Placing the experimental and theoretical deals in confocal view, we had our own contribution of rationales in this quest,[1-3] approaching several case studies, from literature or our own chemical outcome, and proposing useful new tools for structure-property correlations. The main focus is devoted to the f-type complexes, rationalizing the magnetic anisotropy as function of Ligand Field features.

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Morphology and thermo-physical properties of SPS-ed SiC ceramics and composites

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Spark plasma sintering (SPS) was used to obtain dense (>99%) silicon carbide based materials and composites with different morphology. The grains sizes of SiC starting powders have been in the range of (20 nm- 1 micron). Different proportions of micrometric and nanometric powders have been used to optimize the morphology and the thermal properties of final materials. Insertions as W fibers, SiC whiskers and metallic powders (V, Cr, Ti) have been used to realize composites with improved properties. The thermo-physical properties of the specimens were investigated with a Laser Flash Analyser equipment and a dilatometer DIL 402C up to 1000 C. The sample morphology and structure were characterized using a scanning electron microscope and X-ray diffraction. Structural and thermal analyses of bare SiC samples show that nanometric SiC powders are strongly glued together and this process is responsible for enhanced densities and thermal properties, while grain boundaries between nano- and micrometric grains tend to decrease thermal conduction. Metal insertions, including molten metals during the SPS process, contribute to composite consolidations by different mechanisms, depending on the metal nature.

Acknowledgement This work has been carried out within the framework of the EUROfusion Consortium under grand agreement No 633053, WP-EDU.

Functional material depositions inside of glass capillaries; practical aspects and applications

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Many standard technologies used for thin film depositions (e.g. sputtering, evaporation, etc.) are unable to deposit these films on inner surfaces. By proper selection of other technologies, the following materials were successfully deposited inside of glass capillaries: Fe, Co, Cu, Ag, Au, Pt, Conducting polymers, TCO (transparent and conducting oxides) and Photocatalytic oxides (TiO₂). The depositions were performed using the following technologies: Oxidative chemical/electrochemical polymerization (for conducting polymers); Electroless plating (for Cu and Ag); Electrochemical plating (for Fe and Co on pre-existent conducting layers); Thermal decomposition of organo-metallic compounds (for Ag, Au and Pt); Sol gel (for TCO and Photocatalytic oxides). Microfluidic devices were prototyped with these glass capillaries provided with functional material depositions inside of them.

Technological aspects and obtained results will be presented.

Acknowledgement

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Doped BaTiO₃ 1D-nanostructures prepared by template-mediated colloidal chemistryA.-C. Ianculescu¹, C.-A. Stanciu^{1,2}, L. Trupină³, B. S. Vasile¹, R. Trusca¹, M. Cernea³ and A. Nicoară¹¹University "Politehnica" of Bucharest, 1-7 Gh. Polizu, 011061 Bucharest, Romania²National Institute for Lasers, Plasma and Radiation Physics, P.O. Box MG54, 077125 Magurele, Romania³National Institute of Materials Physics, P.O. Box MG-7, Bucharest-Magurele, 077125, Romania

In the present study, the preparation by template-mediated colloidal chemistry, as well as the characteristics of Ce³⁺-doped BaTiO₃ nanotubes and nanowires with the nominal formula Ba_{0.95}Ce_{0.05}Ti_{0.9875}O₃ were described. Porous polycarbonate membranes with channels diameter of 100 nm and 200 nm, respectively, were used as templates. The precursor sol was deposited on both membranes by spin coating. The uncalcined nanotubes obtained by using as template the membrane with channels diameter of 100 nm show an average outer diameter of about 86 nm and an average wall thickness of 9 nm, while, the uncalcined nanoshell tubes obtained by using the membrane with channels diameter of 200 nm show an average outer diameter and wall thickness of 186 nm and 12 nm, respectively. Crystalline Ce-doped BaTiO₃ nanoshell tubes obtained after thermal treatment in air, at 700°C for 1 hour, exhibit a mean outer diameter of 157 nm, higher porosity and larger grains (average grain size of 38 nm) consisting of larger crystallites (of 6 – 9 nm), than the nanotubes with a mean outer diameter of 77 nm, which show grain size of 20 nm and crystallites of 3 – 5 nm. Uniform, uncalcined wires with diameter of about 81 nm were produced by the same method. After calcination in similar conditions the amorphous 1D-structures were converted into crystalline nanowires, with a mean diameter of 60 nm. PFM investigations indicated ferroelectric and piezoelectric characteristics for all the Ba_{0.95}Ce_{0.05}Ti_{0.9875}O₃ nanotubes/nanowires prepared in this study.

Atomic layer deposition of semiconductor oxides on carbon nanomaterialsN. Justh¹, K. László³, B. Berke³, B. Nagy³, G. Mikula¹, L. Bakos¹, Z. Erdélyi⁴, B. Parditka⁴,
Zs. Baji⁵, K. Hernádi⁶, G. Kiss⁶, B. Réti⁶ and I. M. Szilágyi^{1,2}¹Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics,²MTA-BME Technical Analytical Chemistry Research Group,³Department of Physical Chemistry and Materials Science, Budapest University of Technology and Economics,⁴Department of Solid State Physics, University of Debrecen,⁵Institute for Technical Physics and Materials Science, Hungarian Academy of Sciences⁶Department of Applied and Environmental Chemistry, University of Szeged

Our aim was to study the photocatalytic properties of carbon nanostructure/semiconductor oxide composites prepared by atomic layer deposition (ALD). The substrates were fullerene (C₆₀), graphene-oxide (GO), carbon nanospheres, resorcinol-formaldehyde and carbon aerogels. TiO₂, Al₂O₃ and ZnO nanolayers were deposited on them at 80 °C and 160 °C. We followed the preparation and functionalization of the carbon nanostructures and the ALD reactions with TG/DTA-MS, FTIR, XRD, SEM-EDX and TEM measurements. Finally we examined the photocatalytic properties of the samples. The degradation of methyl orange was observed under UV illumination. Unexpectedly, amorphous TiO₂ had photocatalytic activity on these substrates. In summary, a-TiO₂ grown by low temperature ALD can demonstrate photocatalytic activity, which can have considerable industrial impact in the field of photocatalysis.

Mesoporous silica-titania composites as vehicles for oxytetracycline

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Mesoporous silica and titania, biocompatible materials, can be employed as carriers for various biologically active molecules due to their excellent adsorption capacity. Here, we report studies on the preparation of oxytetracycline delivery systems containing various mesoporous silica-titania composite carriers with different antibiotic content in order to establish the influence of structural, textural and support composition on oxytetracycline release profile. The mesostructured silica-titania composites with up to 30%(mol) titania were prepared using tetraethyl orthosilicate and titanium oxychloride as silica and titania precursor, respectively, in the presence of triblock copolymer, Pluronic P123 as structure directing agent. The antibiotic molecules were loaded on support mesochannels by incipient wetness impregnation method using a concentrated aqueous solution of drug. The silica-titania composites and oxytetracycline-loaded were characterized by various techniques: small- and wide-angle XRD, FTIR spectroscopy and N₂ adsorption-desorption isotherms. The antibiotic delivery profiles determined by UV-vis spectroscopy in saline phosphate buffer solution, at 37°C, showed that the increase of titania content in mesoporous composite slowed down the release kinetics. The oxytetracycline-loaded materials showed very good antimicrobial activity against *Staphylococcus aureus* ATCC 25923.

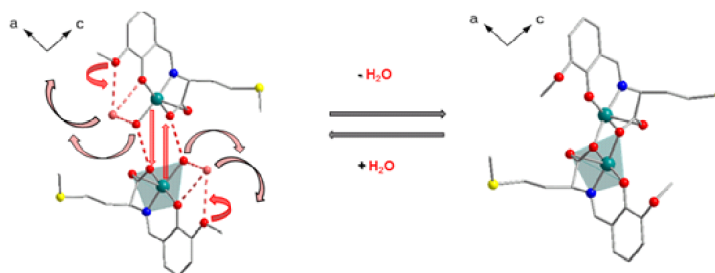
Chirality driven crystallization behavior of tridentate Schiff base complexes

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The most employed strategy for introducing the chiral information into a metal-ion based network consists of choosing of an enantiomerically pure ligand. In this respect, the usage of natural amino acids as chiral precursors is a simple and practical alternative. Moreover, the preservation of amino acid moieties within the resulting ligand can afford both an increased denticity and different kinds of hydrogen bonds that play a critical role in the self-assembly process.

Following this idea, we present herein a chiral monodimensional copper(II) complex based on L- or D-amino acid-containing tridentate Schiff ligand. The dihydrated form, undergoes a single crystal to single crystal transformation to the dehydrated helical double chain, under the influence of heat. The reverse SCSC process involves the regeneration of the original structure under exposure to water vapours. This transformation generates significant changes in magnetic behaviour. Electronic and circular dichroism spectra were also performed according to their relevance for each compound.



Controlling the metoprolol release rate from mesoporous silica-based drug delivery systems

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Cardiovascular diseases are a leading cause of death in the developed world. The development of new drug delivery systems capable of providing controlled drug release over a long time period can improve the efficiency of the treatment. In this study we have designed drug delivery systems for metoprolol, a widely-used β 1-receptor blocker, by employing various mesoporous silica and aluminosilicate carriers. The mesoporous matrices and drug-loaded samples were characterized by small- and wide-angle X-ray diffraction, infrared spectroscopy, nitrogen adsorption-desorption isotherms, thermogravimetric analyses and scanning electron microscopy. Drug loading was performed through a simple impregnation/evaporation method. The *in vitro* drug release profiles were described in terms of the release rates of the burst and steady-state phases as well as the fraction of metoprolol released during the burst stage using a theoretical three parameter model. The effects of the pore size, arrangement, aluminum content and presence of grafted organic groups on the drug release profiles have been identified. The three parameters affecting the release profiles can be judiciously tailored through changing the textural properties of the carriers and the introduction of aluminum or organic groups, resulting in controllable drug release profiles.

Preparation of photocatalytic iron tungstate (FeWO₄) nanosheets and h-WO₃ nanorods by hydrothermal method

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Tungstate oxides and metal tungstates are widely used in catalysis, photocatalysis, gas sensing, as well as in electrochromic applications. Two important representatives, hexagonal (h-) WO₃ and iron tungstate (FeWO₄) are often synthesized by hydrothermal synthesis using sodium tungstate (Na₂WO₄) and hydrochloric acid (HCl) as starting materials, and various additives.

We investigated the effects of different cations in the sulphate additives (Na⁺, NH₄⁺, Fe²⁺, Fe³⁺ salts of sulphate) on the composition and morphology of the products. In addition, we also studied the influence of reaction temperature, i.e. 180 or 200 °C. The products were analyzed by SEM-EDX, XRD, FTIR, Raman, UV-Vis, and their photocatalytic activity was also examined.

In contrast to previous results, Fe(II)WO₄ could be prepared only in the presence of Fe(II)SO₄. In every other case, h-WO₃, Fe(III)₂(WO₄)₃ or other phases were obtained. For the first time we managed to prepare FeWO₄ in the form of nanosheets with a thickness of 20-30 nm and width of 0.5-10 μm. Both as-obtained FeWO₄ nanosheets and h-WO₃ nanorods had good photocatalytic activity.

**New Zn(II) coordination polymers
with *exo*-bidentate ligands assembled in the presence of amino-alcohols**

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The synthesis of coordination polymers with mixed linkers has been attempted not only to generate diverse topologies, but also to give multifunctional systems, and numerous multitopic organic ligands with specific binding strength and directionality have been used. Among them, oxygen or nitrogen containing ligands such as aromatic polycarboxylic acids or bis(4-pyridyl) derivatives have been extensively employed. On the other hand, amino-alcohols have received much less attention, in spite of the variety of coordination modes or their capability for formation of hydrogen bonds.

In the present work we report on the synthesis and characterization of new Zn(II) coordination polymers self-assembled under solvothermal conditions from amino-alcohols and rigid rod-like organic linkers.

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**Monte Carlo simulations
of magnetic ordering in KMnF₃ Ising perovskite structures**

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Transition metal compounds with a perovskite structure represent functional materials, characterized by a variety of particular electronic, magnetic and optical properties.

KMnF₃, as an important member of ABX₃ families, undergoes a transition from paramagnet at room temperature to an antiferromagnetic (AFM) order state.

Monte Carlo Simulations of the Magnetic Behavior (M and χ vs H), Ordering Temperature (T_N), and the calculation of the magnetic exchange coupling constant J , by Ising's simple model of a spin lattice is particularly important for comparison with experiment.

Influence of the crystal structure and composition of nanosize WO₃ on the gas sensing, photocatalytic and catalytic properties

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In gas sensing, photocatalysis and catalysis, up to now only the monoclinic (m-) form of WO₃ has been used. We aimed to explore the properties of the second most important polymorph, i.e. hexagonal (h-) WO₃. We prepared m- and h-WO₃, and we also managed to control their composition, and obtained oxidized (yellow) and partially reduced (blue) m- and h-WO₃ samples. The samples were analyzed by XRD, SEM-EDX, TEM-ED, XPS, ¹H-MAS NMR, Raman and UV-VIS.

We found that in gas sensing both the structure and composition of the WO₃ samples were vital. Oxidized (yellow) h-WO₃ was absolutely selective to H₂S in the presence of H₂, CH₄, NO and CO. When WO₃ was fully oxidized, it always behaved as an n-type semiconductor in sensing NH₃. As a contrast, partially reduced WO₃ samples were n-type only from 200 °C, and p-type below that. In photocatalysis, the composition of WO₃ had the highest importance. The crystal structure had only an indirect effect, as it influenced the composition: m-WO₃ was completely oxidized, while h-WO₃ was partially reduced do to the presence of stabilizing cation impurities. The different composition of m- and h-WO₃ meant different surface properties, and this influenced the nucleation processes when TiO₂ was deposited onto WO₃ by atomic layer deposition (ALD) to yield photocatalytic WO₃/TiO₂ nanofibers, or when catalytic Au decorated WO₃ nanoparticles were obtained by sol-gel.

A new generation of problems in the ligand field modelling. From phenomenology to first principles prediction of optical properties.

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The Ligand Field (LF) theory is often invoked qualitatively for *d*-type complexes, its quantitative approach by parametric phenomenology or ab initio calculations being relatively accessible, though not in simple and routine ways. In turn, the LF on *f*-type elements compounds is yet seen as a complicated domain, not easily accessible, neither with effective Hamiltonian algebras, nor by first principle methods. However, the LF is a very tempting domain, offering interpretation and prediction for optical and magnetic properties. We approach, by analytic handling and non-routine calculations even more complicated problems of the LF in lanthanide based systems, describing inter-shell- *4f-5d* transitions, designing a two-shell LF formalism, proven to be very fruitful in scintillators.

Recycling of vitreous waste in ceramics with thermo-mechanical vocation

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Fused silica offers excellent thermal shock resistance due to its low thermal expansion coefficient ($3.9 \times 10^{-7} \text{ K}^{-1}$, average from 20°C to 320°C), being a proper starting material for obtaining thermal resistant products which during service can withstand strong thermal shocks and corrosion of metal melts.

In this work were investigated the possibilities of recovering vitreous silica waste by using:

- 1) tetraetoxysilane (TEOS) hydrolyzed in basic or in acid environment and
- 2) colloidal silica (SiO_2) in order to preserve high thermal shocks resistance in conjunction with high mechanical strength.

The mineralogical phase evolution was investigated by complex thermal analysis, differential scanning calorimetry, X-ray diffraction and scanning electron microscopy.

The use of vitreous silica wastes in ceramic structures with controlled characteristics by casting-vibrating procedure followed by firing at 1000°C was effective.

The influence of the binder type and the relationship between the applied heating treatment and the thermo-mechanical properties of the specimens is discussed.

The best mechanical strengths of ceramic were obtained with colloidal silica as binder.

SECTION 5

Advanced materials science

POSTERS

Heterotrimetallic ferrimagnetic chains assembled from $\{\text{Cu}^{\text{II}}\text{Mn}^{\text{II}}\}$ binuclear complexes and cyanido metalloligands

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Herein, we report on two new monodimensional heterotrimetallic coordination polymers: $\infty_1[\{\text{Cu}^{\text{II}}\text{Mn}^{\text{II}}\}_3\{(\mu\text{-NC})_3\text{W}^{\text{V}}(\text{CN})_5\}_2]\cdot\text{H}_2\text{O}$ (1) and $\infty_1[\{\text{Cu}^{\text{II}}\text{Mn}^{\text{II}}\}\{(\mu\text{-NC})_3\text{W}^{\text{V}}(\text{bipy})(\text{CN})_3\}][\text{W}^{\text{V}}(\text{bipy})(\text{CN})_6]\cdot 0.75\text{H}_2\text{O}\cdot 1.25\text{CH}_3\text{CN}$ (2), which are obtained connecting preformed $\{\text{Cu}^{\text{II}}\text{Mn}^{\text{II}}\}$ bimetallic nodes by homoleptic $\{\text{W}^{\text{V}}(\text{CN})_8\}$ and heteroleptic $\{\text{W}^{\text{V}}(\text{bipy})(\text{CN})_6\}$ cyanido spacers (H_2L is the compartmental Schiff-base resulting from the stepwise condensation of 2,6-diformyl-*p*-cresol with ethylenediamine and diethylenetriamine). Their X-ray structures and magnetic properties are discussed.

Pyrene behavior in hydrophobically modified sodium polyacrylates without and with surfactants systems

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Water-soluble hydrophobically modified sodium polyacrylates (NaPAC_n) were synthesized by grafting the poly(acrylic acid) (PAA) with 3 % (mol) C_{10} and C_{18} linear alkyl side-chains. The photophysical properties of the NaPAC_n and their mixtures with surfactants were investigated by fluorescence spectroscopy, using pyrene as a probe. Cationic, anionic and nonionic surfactants with the same alkyl chain length (i.e., C_{12}) were employed. The steady-state fluorescence results proved that the sodium polyacrylate (NaPA) does not have hydrophobic microdomains to accommodate pyrene inside. Instead, the NaPAC_n s unveiled intracoil aggregates at a certain polymer concentration which decreases with the alkyl chain length. For aqueous grafted polyacrylate solutions, the dynamic fluorescence proved the existence of both intra- and intercoil aggregates, because the pyrene lifetimes have various values in the different microdomains. The association of polymers with surfactants are strongly dependent on the presence of hydrophobic microdomains and the surfactant nature. Therefore, the hydrophobic interactions play an important role, especially for the NaPAC_{18} – surfactant systems due to the low polarity of the polymer. It was also observed that the cationic surfactant strongly interact with the polymers, while the anionic one hardly did. The nonionic surfactant had an intermediate association behavior.

Synthesis and characterization of Cerium-doped mesoporous bioactive glasses

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The impact of bone diseases and trauma around the world has led to an increased demand for new materials that have applications in therapies for bone pathologies such as restoration and augmentation. Sol-gel derived mesoporous bioactive glasses based on $\text{SiO}_2\text{-CaO-P}_2\text{O}_5$ system with and without cerium as a doping element were investigated. The choice of cerium was related to its low toxicity associated with antimicrobial and antioxidant properties. The microstructure of the bioactive glasses was investigated by scanning electron microscopy (SEM) technique. Pore size distribution and surface area were also determined in order to characterize the textural properties of the samples. The bioactivity of the glasses was tested by soaking them in a simulated body fluid (SBF) at 37 °C for different periods of time. The formation of a hydroxyapatite (HA) layer on the bioactive glass powder was confirmed by XRD, FTIR and Raman Spectroscopy. UV-Vis measurement allowed us to determine the $\text{Ce}^{3+}/\text{Ce}^{4+}$ ratio in the glasses and to correlate it with the hydroxyapatite forming ability. The influence of the bioactive glass composition on the formation of HA layer on the glass powders was established.

Microstructural analysis of NiCrAlY/ Al_2O_3 plasma sprayed coatings after thermal oxidation at 850°C

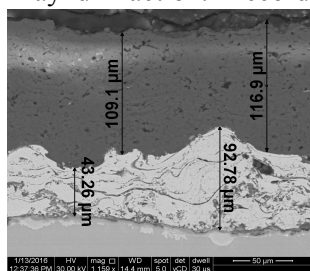
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Nanostructured NiCrAlY/ Al_2O_3 coatings (bond coat/top coat) were deposited on titanium aluminide by atmospheric plasma spray. The isothermal oxidation behavior of double coatings at 850°C for 500 hours was investigated. Effects of isothermal oxidation, in air, on the NiCrAlY/ Al_2O_3 coatings were investigated by scanning electron microscopy with energy dispersive spectroscopy (SEM-EDS) and X-ray diffraction. According to the experimental results, the NiCrAlY/ Al_2O_3 coating shows a good oxidation resistance which is mainly associated with decreased porosity and microcracks. No cracks and delamination occur at the bond coat- Al_2O_3 interface after 500 h of oxidation at 850 °C. In addition, the presence of Al_2O_3 as top coat over the NiCrAlY layer reduces Ni diffusion toward titanium aluminide support and partial pressure of oxygen at the $\text{Al}_2\text{O}_3\text{-NiCrAlY}$ interface and thus prevents the emergence of destructive oxides which require higher oxygen amount to form. No spallation of oxide scale, i.e. no decrease of the mass gain, is noticeable after cooling for the specimen under discussion.



SEM image of coatings

Self-association of some hydrophobically modified sodium polyacrylates in aqueous solution

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Water-soluble associative polymers (APs) are a class of compounds with hydrophilic backbone decorated with a few hydrophobic groups. In water, the reversible association of labels makes APs distinguishable from regular polymers without associative groups and confers them practicability in many fields. The specific behavior of hydrophobically modified sodium polyacrylates (NaPAC_n) is given by the interplay between the electrostatic repulsions of the carboxylate groups and the attractions of the hydrophobic grafts. In aqueous solution, the hydrophobic groups try to avoid the contact with water, and form intra- and inter-macromolecular aggregates. Strong associations are obtained by increasing the alkyl chain length, because the modified polymers are less soluble in water. In this study, we are interested to find out new information on the behavior of randomly modified polyacrylates with linear C₁₀ - C₁₈ alkyl chains, by means of viscometry, steady-state fluorescence and refractometry. It is found out that each NaPAC_n has a characteristic overlapping concentration (c^* - demonstrated by viscometry), which lowers as the grafted chain is more hydrophobic. Steady-state fluorescence unveils intra-coil hydrophobic microdomains, whereas refractive index reveals the existence of both intra- and inter-coil aggregates. The complementarity and agreement between results obtained by different methods is evidenced.

Optical contrast formation in ta-C films by ion implantation

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Tetrahedral amorphous carbon (ta-C) thin films ($d \sim 40$ nm), deposited by filtered cathodic vacuum arc method, have been implanted with Ga⁺ at ion energy 20 keV and ion doses ranging from 3×10^{14} to 3×10^{15} cm⁻². The implantation-induced modification of the films structure causes a considerable change of their optical properties, best manifested by a significant shift of the optical absorption edge to lower photon energies as obtained from the optical transmission measurements. This shift is accompanied by an increase of the absorption coefficient (photo-darkening effect) in the measured photon energy range (0.5-3.0 eV). These results well correlate with those obtained from the complementary ellipsometric measurements in the spectral range of 195-1000 nm. The observed effects could be attributed to additional defects generation and increased graphitization, as well as to gallium colloids formation, as confirmed by scanning electron microscopy measurements. The optical contrast thus obtained between implanted and unimplanted film material could be used for high-density optical data storage using focused Ga⁺ ion beams.

Using dye solutions for studying the wicking in monocomponent textile fabrics

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Radial liquid spreading from an infinite reservoir containing a dye solution onto a horizontal fabric sample was studied. The images of the wet spot during the radial outward wicking were collected with a webcam using an home made experimental set up [1]. The resulting image series were processed with routines especially developed to lead to the area of the wet spot. The time dependence of the wet area gives information about the wicking kinetics and further, by modeling the data, about the possible mechanism. The experiments were performed using solutions of red (rhodamin 6B) or blue (brilliant blue or methylene blue) dyes in linen, polyester or wool samples differing not only by the yarn composition but also by the roughness of the surfaces. The data allow an easy comparison of the textile behavior. Determination of the mass loss of the test liquid might be useful especially for the colored fabrics. Experiments were here conducted upon materials of commercial origin from wool, polyester or cotton. Samples in the original form or deposited with TiO₂ or ZnO were considered as well. All the samples were firstly characterized using complex methods such as optical and scanning electron microscopy, FTIR and diffuse reflectance spectroscopy, XRD, thermal analysis etc. Molecular interactions of the dyes with the specific functional groups, on the textile fibers is evidenced. Methylene blue (MB) has shown a strong interaction with the fabric surface, namely a peculiar behavior among the used dyes. This interaction depends on several factors involving the dye and yarn features in addition to the chemical nature of the fabric.

1. V.F. Cotorobai, I. Zgura, M. Birzu, S. Frunza, L. Frunza, *Colloids & Surfaces A* 497 (2016) 146.

The influence of the oxidation degree of bismuth oxide thin films on their optical properties

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Despite their often complicated structure, bismuth oxide thin films still keep the interest of scientists due to several properties such as: large band semiconducting behavior, with ionic conduction and high refractive index. Thermal oxidation in air is one versatile method that can be used to obtain bismuth oxide from pure bismuth films. But bismuth can form several non-stoichiometric oxides except for bismuth trioxide and the latter exhibits complicated polymorphism and polycrystallinity. This is why in-depth structural analysis is needed in order to properly interpret the other properties of bismuth oxide films. Transmission electron microscopy (TEM) is the method of choice for this purpose. Here we propose a TEM morpho-structural analysis of highly transparent bismuth oxide thin films deposited on glass substrates at two different temperatures, along with the optical study of the chosen films, revealing their high energy band gap, with low sensitivity to the oxidation degree, which, instead, strongly influences their refractive indexes and absorption coefficients.

Tailoring spray pyrolysis deposited thin films for solid state solar cells

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The contribution of photovoltaics (PV) to the electric power production, either in large- or in small-scale systems, is continually increasing. The search for increasing the PVs sustainability over the entire lifecycle lead to novel structures, obtained avoiding critical materials, in less energy-intensive processes. Moreover, the design pre-requisites of different types/generations of PV cells always included increased efficiency and lower costs. Solid state solar cells (SSSC) consist of a solid p-type semiconductor (e.g. Cu_xS , Ni_xS , etc.) acting as absorber which is placed in the n-type semiconductor matrices (e.g. TiO_2 , SnO_2 , ZnO). These are thin film PVs, using very low amounts of active materials.

Following the sustainability pre-requisites, a stacked layered SSSC was obtained using spray pyrolysis deposition (SPD); it consists of a SnO_2 substrate deposited on FTO followed by the active layers: TiO_2 and Cu_xS thin films. Structural, morphological and optical measurements were employed to investigate the properties of the different films involved, in order to create a controlled/optimized interface, as well as to predict and interpret the electrical behavior of the multi-layered structures. By this way, a possible nucleation and growth mechanism was put forward regarding the n-type semiconductor layer(s) in the SSSC. A good structural (cubic) and morphological (fine, spherical grains) compatibility between the SnO_2 and TiO_2 thin films was observed, which was reflected in the electrical properties. This match does not extend to Cu_xS , therefore, an additional porous layer of TiO_2 was added as host n-type matrix.

Polyamine functionalized magnetic nanoparticles for Cu(II) removal from aqueous solutions

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Wastewater from many industries contains toxic heavy metals, which are not biodegradable and tend to accumulate in living organisms, causing various diseases and disorders. Among the heavy metals mentioned above, copper is the most frequently used metal in industries such as mining and petroleum refining. The magnetic separation technology as an efficient purification method has gained increasing attention because of its advantages like easier manipulation of the adsorbents in the presence of a magnetic field and lower energy consumption. To facilitate the adsorption affinity, surface modification has extensively been explored to enable specific metal complexation. In this context, the aim of this study was to synthesize novel magnetic adsorbents functionalized with different polyamines (1,3-diaminopropane, diethylenetriamine, triethylenetetramine) with increased efficiency for Cu(II) ions removal. The synthesized materials have been characterized structurally, morphologically and magnetically. Subsequently, a series of experiments have been conducted to evaluate their adsorption capacity for Cu(II) ions from aqueous solutions and to explore the effect of pH, initial concentration, contact time, on the adsorption efficiency.

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The effect of a “seed” layer upon multi-stage Pulsed Laser Deposition of Aluminum Nitride structures at different substrate temperatures

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We report on multi-stage synthesis of Aluminum Nitride (AlN) on Si (100) wafers, at different temperatures. The first (“seed”) layer was synthesized at 800 °C, the optimum temperature for AlN crystallization. In the second stage, the deposition was conducted at lower temperatures (RT, 350 °C or 450 °C). GIXRD measurements indicate that the two-stage deposited AlN films show a randomly oriented wurtzite-type structure, with nanocrystallites. The peaks are shifted to larger angles, indicative for smaller inter-planar distances. TEM images show that the high-temperature AlN “seed” layer has the role to promote the growth of poly-crystalline AlN structures at lower deposition temperatures. When increasing the deposition temperature, the surface roughness of the samples is of (0.4 – 2.3) nm. Ellipsometry analyses present structures which yield band gap values of (4.0 – 5.7) eV. **Acknowledgements:** LD and INM acknowledge with thanks the support of the Romanian National Authority for Scientific Research and Innovation, CNCS-UEFISCDI, under the project number PN-II-RU-TE-2014-4-1570 (TE 108/2015).

Characterisation of phosphate glasses with magneto-optical applications

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The purpose of present paper is to investigate phosphate glass as vitreous matrix base and doped with rare-earth transition and post-transition ions, as well. The main basic properties of the as-obtained doped phosphate glasses, such as thermal expansion, characteristic temperatures of glasses, density, viscosity, hydrolytic stability were measured. In order to examine potential thin layer properties, scanning electron microscopy (SEM) is employed for evaluation of compositional and crystallization behaviour, and microstructure, as well. The results are discussed in connection with compositions, thermal history, doping elements used in phosphate vitreous matrix.

Chitosan coated-cobalt ferrite nanocomposite for wastewater treatment applications

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Nanocomposite ferrites coated biocompatible polymers are an important class of materials with potential applications as catalysts, sensors/biosensors, adsorbents/microwave adsorbents etc. One of the most frequently used natural and eco-friendly polymers is the chitosan. Due to the presence of a large number of –NH₂ and –OH groups, the chitosan can act as a chelating/gellating agent. The chitosan can chelate toxic pollutants like heavy metals and dyes and has been used for the removal of Pb(II), Cu(II) or Zn(II) ions from the waste waters. The chitosan-coated cobalt ferrite was obtained through one-step *in situ* wet ferritization. The obtained nanocomposite was characterized by XRD, SEM, thermal analysis, FTIR and magnetic measurements. The results on the adsorption process of Pb(II) ions revealed that this nanocomposite is a good adsorbent for lead ions, highlighting its promising potential for applications in the wastewater treatment.

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Nanosized cobalt ferrite synthesis by two soft chemistry methods using Hibiscus extract

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CoFe₂O₄ is a hard magnetic material with high Curie temperature, high coercivity, moderate saturation magnetization, high anisotropy constant, thermal and chemical stability. These specific properties made CoFe₂O₄ a preferred candidate for biomedical applications, waste water treatment, etc. A combination between the soft chemistry methods and the green chemistry is an ideal synthesis strategy in order to obtain ferrite nanoparticles. The use of plant extracts offers the possibility of preparing nanosized cobalt ferrites by a green chemistry approach. The spinel-type cobalt ferrites were synthesized by self-combustion process and wet ferritization reaction using flowers and leaves extracts of *Hibiscus rosa-sinensis*, respectively. The samples were characterized by XRD, SEM, IR, and VSM. The sorption capacity of the cobalt ferrite on Pb(II) ions from aqueous solution was evaluated.

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Graphene hybrids designed for energy storage applications

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Carbon based materials have been widely studied as a new class of energy storage devices and supercapacitors known as electrochemical capacitors. Compared with electrochemical double layer capacitors, pseudocapacitors could provide much higher capacitance and energy density through Faradaic reaction. Transition metal oxides could provide high energy density for pseudo capacitors. It has been found that carbon materials which are combined with pseudo capacitive electrode materials could lead to new materials with enhanced electrochemical capacitance.

ZnO is considered to be a promising material for energy storage applications due to its high specific energy density, non-toxicity and low cost.

In this work, ZnO/graphene composites have been synthesized through solvothermal method. Zn(II)-carboxylic acid coordination polymers have been employed for the synthesis of ZnO particles. Graphene oxide was obtained through modified Hummers's method. The resulted ZnO/graphene composites were characterized by X-ray diffraction (XRD), thermogravimetric analysis (TGA) and scanning electron microscopy (SEM). The electrochemical properties of the composite have been studied by cyclic voltametry (CV) and impedance spectroscopy (EIS). The resulting ZnO/graphene composites exhibited improved capacitive performance compared to the bare ZnO.

On the density functional theory treatment of lanthanide coordination compounds. Challenging the limits with relevant computational experiments.

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The electron structure aspects debated in this work originate from interests related to the molecular magnetism based on the f-type ions, but the general relevance of the current undertaking is larger, concerning the general causal relationships between the bonding regime of lanthanide complexes and properties. The case study touches also methodologic concerns, such as the use of different varieties of Density Functional Theory (DFT) calculations and the encounter of situations nearby the limit of quasi-degenerate ground states. A series of Cu-Ln complexes with a large binucleating ligand has have been investigated by means of density functional theory (DFT) calculations, comparing the Ln=Gd, Tb and Lu. A particular focus has been devoted to the Cu-Tb complex, for which we were able to catch a series of different convergent solutions having relevance for the Ligand Field modelling, in spite of apparent limitations of DFT frame in multiplet problems.

Synthesis and properties of fluorescent 4'-azulenyl functionalized 2,2':6',2''- terpyridinesA. E. Ion^{1,2}, M. Voicescu³, A. M. Madalan², D. Bala⁴, C. Mihailciuc⁴ and S. Nica¹¹"C. D. Nenitzescu" Center of Organic Chemistry of the Romanian Academy, Spl. Independentei 202B, Bucharest²Inorganic Chemistry Laboratory, Faculty of Chemistry, University of Bucharest, Str. Dumbrova Rosie, Bucharest³"I. Murgulescu" Institute of Physical Chemistry of the Romanian Academy, Spl. Independentei 202, Bucharest⁴Physical Chemistry Dept., Faculty of Chemistry, University of Bucharest, Regina Elisabeta 4-12, Bucharest

2,2':6',2''- Terpyridine derivatives are extensively used organic ligands in the field of supramolecular chemistry and material science [1]. It has been established that 2,2':6',2''-terpyridine has low quantum yield fluorescence [2] and significant emission can be achieved after specific modifications of the terpyridine core motif [3]. In this context, the synthesis of tailored terpyridine derivatives with appropriate electron donor/acceptor moieties may allow further improvement of their spectroscopic and electrochemical properties. Novel 4'-azulenyl-substituted terpyridines are efficiently synthesized following Kröhnke methodology via azulenyl-chalcones intermediates. These azulenyl-containing terpyridines show fluorescent emission with the fluorescence quantum yield varying from 0.14 in the case of parent terpyridine to 0.64 when methyl groups are grafted on the azulenyl seven-membered ring. The electrochemical profile contains one-electron oxidation/reduction steps, which can only be explained on the basis of the redox behavior of the azulene unit. In addition, 4'-azulenyl 2,2':6',2''- terpyridine show ability to bind poisoning metal Hg²⁺ and Cd²⁺ cations in aqueous media.

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Citrate-stabilized Prussian blue nanoparticles for biomedical applicationsM. Marin¹, R. Jijie², C. Lete¹, S. Lupu³ and R. Boukherroub²¹"I. Murgulescu" Institute of Physical Chemistry, Bucharest, Romania²Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN), Lille, France³Faculty of Applied Chemistry and Materials Science, University Politehnica of Bucharest

Engineered nanoparticles have attracted a growing interest in the past decade for biomedical applications. The remarkable and unique properties of the nanoparticles have led to the development of nanosized drug delivery systems, magnetic resonance imaging and hyperthermia treatment of tumors, etc. In the present work, we report on the synthesis, photothermal properties and cytotoxicity of citrate-coated Prussian blue Fe₄[Fe(CN)₆] nanoparticles (PBNPs). The PBNPs were synthesized according to a wet chemical method involving the reaction between ferric citrate and potassium ferrocyanide at 55°C. DLS measurements revealed a hydrodynamic diameter of 144 nm of the citrate-coated PBNPs. The UV-Vis spectra showed a broad absorption band with a maximum at 710 nm, providing a possibility for cancer cells ablation under visible-near infrared light irradiation. The temperature of a dispersion containing 0.1 mg/ml PBNPs increased to 50°C (high enough to kill the cancer cells) in less than 150 seconds after exposure to 980 nm laser. The good photothermal properties of the citrate-coated PBNPs suggest their potential application for the treatment of cancer by laser ablation.

Synthesis, characterization, antimicrobial and cytotoxic activity of lanthanide(III) complexes containing the anti-inflammatory drugs isoxicam and tenoxicam

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Six lanthanide(III) complexes with isoxicam and tenoxicam $[\text{Ln}_2(\text{HL})_2(\text{CH}_3\text{COO})_4] \cdot x\text{H}_2\text{O}$ (H_2L = isoxicam, tenoxicam; Ln = Pr, Nd, Gd) have been synthesized and characterized by elemental analysis, IR, UV-Vis-NIR, thermal analysis, magnetic and conductivity measurements. The antimicrobial efficiency of the complexes and the free ligands were examined by in vitro methods against various pathogenic bacterial and fungal strains. The tested compounds were found to possess a more intensive antimicrobial activity against the Gram-positive bacterial strains as compared to the Gram-negative ones. Also, the two ligands, in comparison to metal complexes were screened for their anticancer activity against HT-29 (human colorectal adenocarcinoma) cell line. The results showed a dose-dependent cytotoxic activity of the tested compounds.

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Zinc oxide based TCO's films for solar cell applications

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Nowadays, obtaining ZnO-based materials to be used in p-n junctions is one of the major research directions in the field transparent optoelectronics, including building integrated solar cells.

In the present work, we aim to obtain Zinc oxide-based films with n-type and p-type semiconducting behavior through two chemical methods, on glass supports. The sol-gel method was used to obtain Al-doped ZnO (AZO) films with n-type conduction, followed by the hydrothermal deposition of p-type films with different compositions (N, In co-doped ZnO and Li, Ni-co-doped ZnO). The resulted homo-junctions have been characterized from a structural and morphological point of view by X-ray diffraction and SEM and AFM measurements, respectively. The investigation of the electrical behavior of the structures was done using Hall effect and I-V measurements.

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Synthesis of Mn-doped ZnO nanostructures by chemical methods

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Synthesis of ZnO nanostructures with controlled size and shape is very important in controlling their physical and chemical properties, and crucial for their potential uses.

In the present work we propose to obtain Mn-doped ZnO nanostructures with Mn atomic concentration of 1%, 2% and 5% by sol-gel process and hydrothermal method. In sol-gel synthesis, thermal treatment of the as-prepared powders at 500°C for 1 h led to Mn-doped ZnO nanostructures. Through the second method, instead, nanocrystalline structures of Mn-doped ZnO were directly obtained during the synthesis process. The obtained powders were studied by thermogravimetric analysis (TGA), differential thermal analysis (DTA), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR) and scanning electron microscopy (SEM).

These Mn-doped ZnO nanostructures appeared promising materials for harvesting applications.

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New precursor method for $\text{CoFe}_{2-x}\text{Cr}_x\text{O}_4$ spinel oxides

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Nanosized chromium substituted cobalt ferrites ($\text{CoFe}_{2-x}\text{Cr}_x\text{O}_4$) have received attention due to their applications as high density information storage, ferrofluids, biomedical treatments, pigments and catalysts. $\text{CoFe}_{2-x}\text{Cr}_x\text{O}_4$ ($x = 0.0, 1.0, 1.5$) were synthesized by a wet chemistry method – the precursor route *via* gluconate precursor decomposition. The complex precursors have been characterized by chemical analysis, FTIR, UV-Vis and thermal analysis. The final oxides were investigated by XRD, SEM, FTIR, Mössbauer spectra and magnetic measurements.

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Synthesis of pure-phase W_2C -Pd(0) nanocomposites as potential electrocatalysts for formic acid oxidation

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Unlike the direct synthesis of W_2C from elements, taking place in a narrow concentration range above 1250 °C, we report a facile Pd(0) catalyzed carbothermal reduction method, which can be employed at temperatures of 600-1000°C and any C:W ratio above stoichiometric minimum. Using a macroporous C source, the method yields pure-phase W_2C with particle sizes less than 500 nm. A W:Pd ratio of 5 or lower (at.) was found to yield pure phase semicarbide. The carbothermal reduction reaction was studied by thermogravimetry-calorimetry methods, while the obtained samples were characterized by X-ray diffraction, XPS and SEM-EDX. The resulting materials were investigated by cyclic voltammetry and chronoamperometry as anodes for the oxidation of formic acid in proton exchange membrane fuel cells. The W_2C -Pd/C composite show similar current densities and improved stability with respect to commercial Pd electrocatalysts, being suited for formic acid electro-oxidation.

SiO₂-ZnO coatings for preservation of historical glasses

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The preservation of historical items is an important subject developed worldwide. The historical objects from glass contain small quantities of transitional elements as Cu, Mn, Fe that decrease their chemical stability. They were added for obtaining different colors. Previous studies reported the protection of the historical glasses by coating with silica or SiO₂-ZrO₂ thin films. The historical glass items deterioration is determined mainly by weathering and bacteria. ZnO is used in different materials as antibacterial, UV-protection or self-cleaning agent. In order to protect and improve the surface of historical glasses, we design appropriate SiO₂-ZnO based coatings and studied their structure and properties. The chemical stability of model glasses that reproduce historical ones and coated model glasses were established.

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1D and 2D ZnO and Al:ZnO interconnected nanostructures for sensing applications

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1D and 2D zinc oxide (ZnO) nanostructures with excellent electrical and optoelectronic properties are targeting high-performance devices such as field-effect transistors, sensors, photovoltaics, light-emitting room temperature UV lasers.

The paper presents hydrothermal synthesis of interconnected 1D (nanorods, nanowires) or 2D (nanosheets, nanowalls) ZnO and Al-doped ZnO nanostructures integrated directly into functional devices (UV sensor) with two terminals by localized growth on patterned substrate with interdigitated metal electrodes. The dimensions and distances between electrodes were designed in correlation with the size of nanostructures (1.5, 5 and 10 μm). The localized growth of nano/micro interconnected wires and/or sheets in the electrodes region was achieved by delimitation in PMMA (electron resist) of growing area in the region of metal electrodes by electron beam lithography (EBL). The I-V (current-tension) characteristics of the nanostructures connected to metallic electrodes were measured in dark and under UV radiation and in different gasses atmosphere.

Key words: *hydrothermal synthesis, (Al)ZnO, nanowires & nanorods, nanosheets, sensors*

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Characterization of the pure halogenated thiourea derivatives and their host-guest interactions with 2-hydroxypropyl- β -cyclodextrin in solid state and in aqueous solution

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N-(p-chlorophenyl)-N'-(2-thenoyl)-thiourea (I), N-(p-bromophenyl)-N'-(2-thenoyl)-thiourea (II), N-(p-iodophenyl)-N'-(2-thenoyl)-thiourea (III) are new synthesized 2-thiophenecarboxylic acid thioureas and they showed antimicrobial activity against bacterial and fungal strains. The above compounds come to offer significant advantages in future treatment strategies; still, the use of these compounds is limited because of the poor solubility. The aims of this study are to characterize the pure compounds and to evaluate the host – guest interactions between thioureas (I), (II) and (III) and 2-hydroxypropyl- β -cyclodextrin (HP- β -CD) in solid state by differential scanning calorimetry (DSC), thermogravimetry and Fourier transform-infrared spectroscopy (FTIR) methods and in aqueous solution by UV-Vis spectroscopy and dynamic light scattering (DLS). “Melting in solution” complexation method was used to obtain the solid complexes and the resulted data indicate the occurrence of a complete encapsulation of active drugs (I), (II), (III) in HP- β -CD cavity for 2:1 of host : guest molar ratio. For the first time the decomposition kinetics of pure compounds (I), (II) and (III) in solid state obtained by DSC in nonisothermal conditions using different heating rate and the FTIR, UV-Vis and DLS data for pure compounds were reported. The values of the enthalpy 49 kJ/mol, and activation energy 94.5 kJ/mol of the decomposition for the compound (II) are slightly higher than those of compounds (I) and (III).

Influence of hydrophilic polymer on polysulfonic membrane properties: Rheological and microstructural aspects

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Development of new polymer materials represents one of the important elements required for improvements of membrane performance and their properties, such as antimicrobial, biocompatibility, and environment stimuli responsive. Quaternized polysulfones (PSFQ) have received widespread attention, being used as membrane materials due to their special properties. On the other hand, the polymers blend concept significantly improves the properties of membranes. In this context, the cellulose acetate phthalate (CAP) was chosen as hydrophilic modifier and pore-forming agent, capable to improve the performance of the PSFQ membranes for biomedical applications. Particularly, the rheological study of PSFQ/CAP blend in N-methyl-2-pyrrolidone (NMP) is essential for better understanding of the phenomena developed by the polysulfone films. The changing trend in films morphology can be associated with the different chain conformation modifications (described through the rheological behavior from the non-linear flow curve) due to the addition of flexible and hydrophilic groups of CAP in the casting polysulfonic solutions, and implicitly, the cumulative effects of the specific interactions present in system. Therefore, the results of this work will provide insight on the development of high-performance membranes for subsequent researches in biomedical field.

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On exchange coupling and bonding in the Gd₂@C₈₀ and Gd₂@C₇₉N endohedral dimetallo-fullerenes

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A series of computational experiments performed with various methods, on the issue of bonding regime and exchange coupling in the title compounds. The Gd₂@C₈₀ is computed with a very weak exchange coupling, the sign depending on the method, while the Gd₂@C₇₉N has resulted with a strong coupling and ferromagnetic ground state, irrespective the computational approach. No experimental estimation exists, but the ferromagnetic groundstate of Gd₂@C₇₉N is confirmed from paramagnetic resonance data. The theoretical simulations are saving resources and effort, given the fact that the chemistry of endohedral lanthanide complexes is very difficult producing only small amounts of sample, insufficient for complete measurements.

Synthesis of CeO₂- SiO₂ mesoporous materials for CH₄ total oxidation

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The aim of the present work was to establish the effect of Ce addition on mesopore structure, morphology and catalytic properties of CeO₂-SiO₂ composites in the total oxidation of CH₄ in air. CeO₂/SiO₂ mesoporous materials were prepared by sol-gel method. The starting synthesis precursors were tetraethoxysilane as SiO₂ source, cerium nitrate as cerium precursor, Pluronic P123 as templating agent and ethanol as solvent. A series of mesoporous ceria-silica composites with Ce/Si molar ratio between 0.05 - 0.4 were obtained and characterized by X-ray diffraction, thermal analysis, N₂ adsorption-desorption, scanning electron microscopy, transmission electron microscopy, temperature programmed oxidation (TPO), Raman and FTIR spectroscopy.

The catalytic properties of the samples were tested in the complete oxidation of CH₄ in air, between 200 and 550 °C. The obtained materials are active in complete oxidation of methane in air. A significant effect of ceria on catalytic activity was evidenced, as conversion of methane increases with ceria content. The comparison between TPO results and catalytic tests shows that the maximum conversion of methane coincides with the absorption of oxygen. The catalytic activity of the mesoporous CeO₂-SiO₂ powders stems from the oxygen vacancies of both oxides. We propose that the emission of oxygen at 300-400°C is the result of oxygen migration and of restoring the oxygen vacancies in oxidized cerium(IV) oxide. These species are considered to determine the catalytic activity in the total oxidation reaction of methane.

New Zn(II) coordination complexes as precursors for ZnO photocatalysts

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In recent years, thermal decomposition of coordination complexes has become a suitable way for preparation of metal oxides with improved properties for various applications. The potential of Zn(II) molecular compounds as precursors for ZnO phases has been investigated and it has been shown that particles with controlled morphologies could be generated by the appropriate choice of both the starting compound and the thermal treatment.

In the present work we report on the obtaining of ZnO nanomaterials from Zn(II) binuclear compounds and their photocatalytic activity for degrading endocrine disrupting chemicals such as Bisphenol A.

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Morphological and structural characterization of oxidic nanopowders

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Investigates of nanostructured materials elaboration are one of the most important topics at present due to the applications in all the fields of our life: electronics, aeronautical industry, medicine, foods or defense. Our research was motivated by the fact that in nanometric domain the crystal structure and mechanism of transformation of pure and doped oxide is depending by elaboration method. In our article the influence of elaboration method on the morphological and structural characteristic of nanostructured zinc and manganese oxides has been studied. Different fabrication techniques such as mecnanosynthesis, metal organic chemical vapor deposition, spray pyrolysis, ion-beam-assisted deposition, laser ablation, sputter deposition, template-assisted growth, precipitation, hydrolysis, pyrolysis and hydrothermal methods have been developed for nanoxides powders preparation. To offer an alternative to mechanical chemical processes for the manganese and zinc oxide nanopowders elaboration the present study focuses on the physical synthesis using solar energy. The Solar Physical Vapor Deposition (SPVD) is an original process to prepare nanopowders using solar reactors working under concentrated sunlight in solar furnaces. The morphological and structural characterization were completed using XRD, SEM, XRF and EDS.

Study of tricalcium silicate (alite) as solid solution with SnO₂

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This research was required, from the industrial perspective, to study the feasibility of the replacement of raw materials for cement production with alternative materials containing trace amount of tin like, fly ash, refuse derived fuels, plastics or waste from steel polishing. Tin may modify the temperature of the first liquid phase formation and/or the amount of the melt, alter the viscosity and surface tension of the melt, affect both crystal growth and morphology and change the rate of the reactions occurring in the solid state within the liquid phase or at the liquid–solid interface. The effect of tin oxide on the formation of solid solutions with tricalcium silicate were synthesized for this study. The formation of hydroxy-stannate during the hydration reaction of alite doped with Sn is important from the protection against corrosion. The samples were analyzed by thermal analysis, X-ray diffraction (XRD) and scanning electron microscopy coupled with energy dispersive X-ray spectroscopy (SEM-EDS).

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Synthesis of thin nanostructured films by plasma polymerization for humidity sensors application

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Thin plasma polymers were synthesized by capacitively coupled radio frequency glow discharge under different operating conditions of glow discharge current density, monomer flow rate, polymer film thickness and modification of the polymer surface in an ammonia plasma. The chemical structures of the obtained nanomaterials were investigated by FTIR spectroscopy. The spectroscopic study revealed that the plasma parameters significantly influence the chemical structure of the polymers. The influence of the same parameters on the humidity sensing properties of the polymers is studied by a quartz crystal microbalance (QCM). The sensitivity of the films to humidity detected by polymer-QCM system was enhanced by working at the highest current density and monomer flow rate and by raising the film thickness and exposure to the ammonia plasma. The results are very promising for development of thin plasma polymer film - QCM systems suitable for humidity (from 20 to 100 % relative humidity) sensors.

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The effect of borax upon Sodium dodecyl sulfate - Poly(acrylic acid) association

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Aqueous solution interactions between polymers and surfactants represent a great interest topic, due to their use as colloidal systems stabilizers, rheology modifiers, emulsifiers or flocculating agents in products such as cosmetics, food, medicines, detergents or paints. Inorganic salts can moderate the electrostatic effect influencing the surfactant-polymer association. On the other hand, borax has found applications in a large diversity of fields including detergents, soaps, medicine, optoelectronics, hydraulic fluids for oil recovery, metallurgy, ceramics and glass, insecticides, etc. In this study we evaluated borax's effect upon sodium dodecyl sulfate (SDS)-poly(acrylic acid) (PAA) complexes. Comparison was made by using both unmodified and fluorescently modified polymers. Also, the effect of sodium chloride versus borax on the polymer-surfactant complexes was followed. To this end, a poly(acrylic acid) with molecular weight of 25000 was grafted with 2.4 % 1-naphthylmethylamine (PAA25Np42). Surface tension, and conductivity measurements revealed that both naphthyl tag and borax reinforce the interaction between SDS and polymer. The photophysical data (polarity index, excimer formation and lifetimes) obtained from steady-state and time-resolved fluorescence measurements gave insight on the nanostructures formed between the weak polyelectrolyte and the anionic surfactant.

Studies on SrO mesoporous silica for drug delivery

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In this study we incorporate strontium (Sr^{2+}) into mesoporous SiO_2 in order to develop a bioactive Sr-Si mesoporous glass with the capacity for drug delivery. We investigated the effect of Sr^{2+} on mesoporous structure and its suitable properties for drug delivery applications.

A series of mesoporous SrO- SiO_2 species with different chemical compositions were prepared by a template-induced self-assembling method. As SiO_2 source, tetraethylortosilicate (TEOS) was used in the presence of Pluronic 123 (Triblock copolymers based on poly(ethylene glycol)-poly(propylene glycol)-poly(ethylene glycol)) template agent. The chemical and structural characterization of the obtained materials was realized by X-ray diffraction, scanning electron microscopy, transmission electron microscopy, thermal analysis, specific surface measurements and pore size distribution.

Doxycycline, a tetracycline antibiotic, was chosen as a model drug because of its tendency to form complexes with alkaline earth elements. The in vitro release profiles, obtained in simulated body fluid at 37 °C show that Sr-containing samples are more suitable to act as sustained release doxycycline delivery systems than pristine mesoporous silica. The doxycycline release profiles can be controlled by adjusting the Sr fraction in the SrO- SiO_2 glasses.

Substrate temperature effect on the structural and optical properties of ZnSe thin films

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ZnSe thin films were deposited onto glass substrates by vacuum thermal evaporation technique. The substrate temperature was varied from 300 K to 473 K. The films structure was studied by means of X-ray diffraction technique. The film crystallites are preferentially orientation with (111) planes parallel to the substrate surface. The surface morphology was investigated by vertical-scanning interferometry. The average roughness and root mean square roughness were calculated. The optical properties of tin oxide thin films were investigated using spectrophotometric measurements of transmittance and reflectance in the wavelength range 300-1100 nm. The transmission and reflection spectra were used to determine the absorption coefficient, α , and optical band gap energy, E_g , of ZnSe thin films. The optical band gap decreases from 2.67 eV to 2.55 eV when the substrate temperature increases from 300 to 473 K.

Novel lipoic acid@SiO₂@Ag nanocomposite: Synthesis, characterization and evaluation of antimicrobial, cytotoxic and cell cycle modulatory effects

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A novel nanocomposite Lipoic acid@SiO₂@Ag has been synthesized by the covalent immobilization of lipoic acid on the Ag nanoparticles-decorated SiO₂ nanospheres. The hybrid material obtained was fully characterized by FTIR, TEM, SEM, UV-Vis, XPS and TG. Its antioxidant, cytotoxic, antimicrobial activities and the influence on mammalian cells cycle were evaluated. The results of this study indicated that the immobilization of lipoic acid on SiO₂@Ag induces an enhanced specificity of interaction with different mammalian cell lines and increased antioxidant activity. On the other hand, the cytotoxicity and antimicrobial properties of the novel composite are not improved in comparison with the SiO₂@Ag. This behavior could be attributed to the significant antioxidant potential of the lipoic acid that protects the bacterial cell from the bactericidal activity of Ag by maintaining the antioxidant status of the cell.

Ceramic materials based on doped barium strontium titanate

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Ceramics based on barium strontium titanate are doped to modify the structure and improve the dielectric properties of the ceramic. Mg doped Ba_{0.5}Sr_{0.5}TiO₃ (BST) ceramics were prepared by solid state reaction using BaCO₃, SrCO₃, TiO₂ and MgCO₃ as raw materials (reagents). Magnesium was chosen as dopant because of the value of the ionic radius ($R_{Mg^{2+}} = 0.72 \text{ \AA}$) comparable with the ionic radius of titanium, which it substitutes, $\sim R_{Ti^{4+}} = 0.605 \text{ \AA}$. The ratio for Ba_xSr_{1-x}TiO₃ was chosen $x=0.5$ because at this ratio $T_{curie} \sim 243 \text{ K}$ (-30°C). At room temperature and at $t^0 > -30^\circ\text{C}$ this ceramic has a cubic paraelectric structure, ideal for application in microwaves. The X-ray diffraction analysis (XRD) suggested that the optimal processing temperatures range between 1300°C and 1400°C . At lower sintering temperature, such as 1200°C , and at higher sintering temperature, such as 1450°C , a secondary phase appears identified as barium orthotitanate: Ba₂TiO₄. Scanning electron microscopy (SEM) analysis showed up that the average grain size reduces and the porosity percentage raises when the ceramics are doped, in this case with magnesium. For the doped ceramics, the change of the dielectric behavior was studied by impedance spectroscopy.

SECTION 6

Biophysical, environmental and green chemistry

KEYNOTES

Formulation of a nano-emulsions-based system for loading and releasing of Ketoprofen

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The growing demand of more efficient medicines forces to adapt drug delivery systems because of the low solubility of many active pharmaceutical ingredients in biocompatible solvents. Different strategies have been developed to overcome this drawback and one of the most popular approaches is the entrapment of a drug molecule into inert vehicles. Various systems based on micelles, microemulsions, emulsions and even inorganic materials, have been formulated for this purpose. Here, a new nanocarrier for loading and releasing of drugs is reported and ketoprofen was used as a model drug. More precisely, the carrier is a hybrid material prepared by combining O/W nano-emulsions, into which the drug has been solubilized, with mesostructured silica. This organic-inorganic hybrid material shows a controlled release of the drug, depending on pH. If the drug is impregnated into the bare hierarchical meso/macroporous dual silica material, obtained after removal of organic components by extraction, only 8 wt.% of ketoprofen is released in a phosphate buffer media (pH 7.4), probably due to its low solubility in the aqueous phase. The drug solubility and the release strongly increase by adding Pluronic micelles in the receptor phase, suggesting a micelle-promoted and assisted release mechanism. Whatever the vehicle, a pseudo-Fickian release mechanism is observed. Moreover, the release of ketoprofen is better controlled from the hybrid nanocarrier than from the hierarchical bare porous silica.

Influence of synthesis parameters on characteristics of KIT-6 type ordered mesoporous silica as support in photocatalytic and biocatalytic reactions

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In this paper we varied the synthesis conditions (temperature of the hydrothermal treatment, alcohol cosolvent and surfactant) of KIT6 mesoporous silica with three-dimensional cubic Ia3d symmetry. Using a quaternary mixture of surfactant (P123, Triton X 100), demineralized water, HCl (37%), a siliceous precursor (TEOS) and a certain alcohol, it was possible to obtain mesopore sizes varied between 3-11.5 nm. The obtained materials were characterized by X-ray diffraction, N₂ adsorption-desorption, SEM and TEM microscopy and UV-Vis spectroscopy. The KIT6 samples with higher porosity, surface area, high ordered porous structure and morphology were selected as supports for immobilization of metals by impregnation and enzymes after pretreatment of silica with glutaraldehyde. The obtained photocatalysts (Ti-KIT6 modified with Ce and Pt) and biocatalysts (laccase-KIT6) were tested in organic pollutants degradation (catechol, methyl orange) from water. Photocatalytic reactions were carried out at room temperature in neutral pH conditions. The obtained results evidenced a higher activity of samples modified with cerium oxide in degradation of methyl orange. The obtained laccase-KIT6 biocatalysts were tested in oxidative degradation of catechol. A higher activity was obtained for samples with covalent binding of laccase. In conclusion, all the photocatalytic and biocatalytic tests evidenced the effect of synergism between silica support and metals or enzyme active sites on catalytic performances.

The extent of albumin denaturation induced by aliphatic alcohols: an EPR study

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Various physico-chemical factors such as heat, high or low pH, or exposure to organic solvents can induce reversible or irreversible changes of proteins conformations.

The aim of this study was to investigate the effects of alcohols on the conformation of protein as revealed EPR spectroscopy. It is well known that fatty acids and compounds with similar structures bind strongly to albumins. In our study, we used two spin probes bearing a linear hydrophobic tail: 5-DOXYL stearic acid and 4-(N, N'-dimethyl-N hexadecyl) ammonium-2,2',6,6'-tetramethylpiperidine-1-oxyl iodide (CAT16). The analysis of EPR spectra reveals that the presence of some alcohols influences the binding of the spin probes to the albumin. A complementary method, the circular dichroism spectroscopy was used to establish if the alcohols replace the spin probes from their complexes with albumin or induce conformational changes.

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Green synthesis, antimicrobial behaviour and DFT studies of selected benzimidazoles

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Benzimidazole compounds represent one of the main biologically active classes cited in literature. A green, one-pot, free-solvent synthesis of biologically active 2-substituted benzimidazoles was achieved. New N-Mannich bases were synthesized from benzimidazoles, secondary amines and formaldehyde. The structures of all compounds were confirmed by ¹H-NMR, FTIR data and elemental analysis. All benzimidazole derivatives were evaluated by qualitative and quantitative methods against 9 bacterial strains. A DFT analysis of molecular structure and frontier molecular orbitals HOMO-LUMO was performed using the GAMESS 2012 software. Antimicrobial activity was correlated with electronic parameters (chemical hardness, electronic chemical potential, global electrophilicity index), Mullikan atomic charges and geometric parameters of the benzimidazole compounds were calculated with GAMESS. It has been found that the planarity of the compound, symmetry of the molecule and the presence of a nucleophilic group are advantages for a high antimicrobial activity.

SECTION 6

Biophysical, environmental and green chemistry

POSTERS

Novel aminopyrazole derivatives biologically active. Structural analysis.

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In this paper we report the synthesis and characterization of some new substituted N and N,N-bis-[(1H-pyrazol-1-yl)methyl]-halogenophenylamine that exhibit potential antibacterial and antitumor activity. For a deeply understanding of the possible mechanism and properties, we perform a structural analysis by means of single crystal X-ray diffraction and theoretical approaches. (Fig.1.)

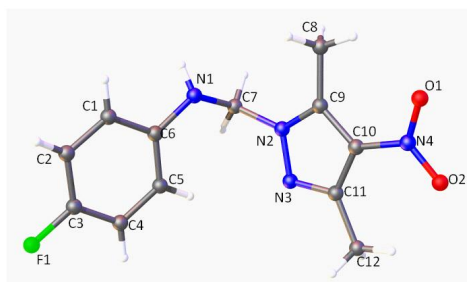


Figure 1. Molecular structure of N-[1H-3,5-dimethyl-4-nitrophenyl-1-yl)methyl]-fluorophenylamine.

Investigation of microbial degradation of keratin substrates with optical and electron microscopy

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Keratin, the major component of hair, feathers and wool is characterized by a high stability and resistance to enzymatic degradation due to the extensive disulfide bonds and cross-linkages. Therefore, keratin substrates are water insoluble and their accumulation mainly in the form of feathers and hair from various industries generates waste disposal problems. The utilization of keratin-degrading microorganism may represent a method to reduce the environmental pollution, also to recycle of keratin wastes. The aim of present study was to investigate the ability of several keratinophilic fungi to degrade keratin substrates. Direct observations of keratin substrates before and after the contact with keratinophilic fungi using optical and electron microscopy techniques lead to useful information regarding the microstructure of samples. Morphological modifications of substrates were observed, such as cuticle lifting and exfoliation of hair strand. A relationship between microstructure and degradative potential of tested fungal strains was evidenced.

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Polyampholyte complexes with variable copolymer architecture examined by Monte Carlo simulations

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We have addressed the electrostatic-driven complexation at the stoichiometric charge ratio of a linear charged homopolymeric chain and an oppositely charged copolymers with different topologies. Strong polyanions as well as a library of copolymers differing in terms of the neutral monomer fraction of the copolymer were examined, and three different architectures (branched versus multiblock versus random) were modelled using a coarse-grain approach at each copolymer composition. The compaction of polyanion by the branched and multiblock copolymers resulted in a core-shell conformation and a structureless spherical complex was found in the presence of the random copolymer. Upon increasing the fraction of neutral monomer, a gradual transition from a globular structure to an extended one was found out only for branched and multiblock copolymers, with the random copolymer providing the largest degree of compaction among the three copolymer types at high fraction of neutral monomer.

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KIT-6 mesoporous silica nanoparticles as support for enzyme immobilisation

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In this work, we are reporting the synthesis of biomaterials with catalytic properties by immobilization of laccase on KIT6 mesoporous silica with cubic arrangement of mesopores. The effects of KIT6 mesoporous silica porosity and morphology on yield enzyme immobilization and catalytic properties were evidenced. KIT6 mesoporous silica with ordered porous structure, have been synthesized at different synthesis conditions by using pluronic P123, as structure-directing agent, in acidic medium and various alcohols. The obtained materials were characterized by XRD, N₂ adsorption-desorption and SEM/TEM microscopy. The influence of synthesis temperature on pore diameter, surface area and pore volume of KIT6 materials was evidenced. The selected supports were thereafter functionalized by a post-grafting procedure with aminopropyltriethoxysilane-APTES and characterized by TGA, X-ray diffraction, N₂ adsorption-desorption, SEM and TEM microscopy and FTIR spectroscopy. The laccase was linked on support by physical adsorption, using KIT6 supports, and covalent binding on KIT-NH₂ or KIT6 pretreated with glutaraldehyde. The higher yield of laccase immobilization and activity was obtained for biocatalysts obtained by covalent interaction of enzyme. For the same support the immobilization yield of lacase increases with time of pre-treatment with glutaraldehyde.

Althaea officinalis L. supported on SBA-15 MSN as new biohybrid delivery vehicle

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Althaea polysaccharides (radix, folium and flores) are used as active ingredients but also additive or excipients in pharmaceutical industry. We report here a successful and efficient method for the immobilization of Althaea folium extracts on SBA-15 mesoporous silica nanoparticles (MSN). Althaea polysaccharides were obtained by extraction from folium in neutral or acidic conditions of aqueous solution. After extraction process and immobilization, the polysaccharides were identified by different techniques (TGA, UV-Vis, XRF, EDAX). The elemental composition shows the presence of C, O, K, Ca, S, Mg and P as main compounds. TGA and EDX analysis revealed that the immobilization was done successfully with the preservation of the SBA-15 silica structure. The higher concentration of Althaea folium on SBA-15 was obtained in case of the extract obtained in acidic conditions. The HPTLC studies confirmed the immobilization of active constituents and their viability was evidenced by confocal microscopy. The results suggests that the mesoporous silica nanoparticles can be used as a delivery vehicle for Althaea polysaccharides, which made them highly promising in biomedical applications.

Thermal stability of two PEG-epoxy composites as candidates for thermal energy storage materials in buildings

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Polyethylene glycol-epoxy, PEG-EP, composites obtained by mixing a PCM component (PEG of molecular weights of 1500 and 2000) with epoxy resin (EP) and Al powder, were investigated with respect to their application as thermal energy storage systems (TES) in nearly zero energy consumption buildings (NZBs). Maintaining of thermo-physical parameters of PCMs over years enables long lasting building elements. Thus, thermal stability of the PEG-EP composites was assessed by (i) kinetical investigation of the solidification processes of the aged samples, (ii) *in situ* μ -Raman spectra during phase change processes (i.e. melting/freezing processes) and (iii) monitoring of the structural changes induced by UV irradiation in a UV-DSC system. Thus, the longer chain in the PEG 2000-EP, the more damaged chain structure is present under UV exposure. PEG component with higher molecular weight of 2000 is biased to UV degradation and hence unusable as building element with direct sun exposure. However, almost unchanged thermal and structural behavior was depicted for naturally aged PEG-EP composites under discussion. Therefore, good stability of these composites means prolonged life in service.

Novel ZnO composites synthesized *via* polysaccharides-assisted methods

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The synthesis of advanced materials through green synthetic procedures that use as much as possible moderate reactions conditions, convenient in terms energy consumption and nontoxic, cheap bio renewable raw materials, is one of current materials science task. One way to fulfill this goal is the employment of biomass and/or constituent carbohydrates as reaction additives in the synthesis of various materials with applications in diverse areas of great importance [1].

A bioinspired one-pot approach for the synthesis of ZnO–carbohydrate hierarchical architectures was developed. The synergy between a saccharide (mono-, di- or polysaccharide) that contains D-glucose units and triethanolamine is the key parameter of the synthetic methodology. The morphology of the ZnO composites is dictated by the saccharide used, and rod, spindle, solid and hollow spherical-like ZnO structures are obtained by varying the carbohydrate.

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ZnO and ZnO-carbon composites obtained through alginate gel template methods

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Alginate is a natural block polymer of the uronic acids, negatively charged, derived from brown seaweed (an abundant, renewable, and nontoxic biomass). It is an unbranched polysaccharide that contains blocks of polyguluronate (-G-)_n, polymannuronate (-M-)_n and alternating (-G-M-)_n units in varying proportions depending on the source species of seaweed. Several important properties recommend polysaccharide alginate for the use in materials synthesis [1].

Alginate ionotropic gel formation that defines a confined space for cation localization was used to obtain suitable precursors for metal oxide and metal oxide-carbon composites. In this gel, the cation acts as crosslinker between two adjacent polymer chains. The poly-G blocks are mainly responsible of such ionic interactions, as in the presence of multivalent cations they can associate to form aggregates of the “egg-box” model of ion binding. The transformation was monitored by thermal analysis coupled with FT-IR and the obtained materials were analyzed by FT-IR, XRD, UV-VIS, PL, BET and SEM measurements.

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Synthesis and electrochemical studies of some indolizine derivatives

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The indolizine is a new class of promising molecules to be used in optoelectronic devices and biomolecular labeling. The syntheses of some indolizine derivatives and their photophysical properties, due to the strong fluorescence in the UV-visible region, have been already investigated but only a few electrochemical properties of indolizines have been described. They can be involved in the formation of redox active films with medicinal and pharmaceutical applications.

The electrooxidation of indolizine in acetonitrile/ KClO_3 was studied using cyclic voltammetry (CV-Bio-logic SP 150). The cyclic voltammetry studies have shown evidences of redox process as decisive factor in the intramolecular cycloaddition forming indolizines during oxidation. The differences in voltammograms are attributed to the differences from functional group and electron transfers.

keywords: Electrochemistry; Cyclic voltammetry; Indolizine

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Characterization by Fourier transform infrared spectroscopy (FTIR) and elemental analysis (EA) of the products obtained from biomass gasification

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The aim of this study was to determine the transformations during thermal treatment of meat processing residues under non-oxidant conditions with respect to their chemical compounds. Representative samples were processed in a tubular oven. The influence of process temperature on product transformation during pyrolysis treatment and the kinetics of pyrolysis phase were investigated. After experimental tests were conducted at various temperatures in the range of 300⁰C - 500⁰C, solid and liquid reaction products were sampled. The resulting char was subjected to full calcination process and ash fraction was collected.

The reaction products were characterized by ATR-FTIR spectroscopy. Both the degradation of aforementioned compounds and the formation of new compounds resulted from this process was pursued. The results were corroborated with data obtained by elemental analysis (EA) for the same compounds. The research revealed the influence of processing temperature on the chemical compounds present in the reaction products as well as the potential of meat residues as renewable energy source for derived fuel production through thermochemical conversion.

Evaluation of drinking water quality in Galati county achieved by monitoring some physical and chemical parameters

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This study investigated the seasonal variations in drinking water quality parameters. These variations are important for evaluating temporal variations of water pollution. For this purpose we collected samples from Călmăţui and Cuca, two villages in Galaţi County. Galati is an important city in Romania at the longitude of 28 and latitude of 45.4. The distance between Cuca and Galati is 37 km and between Călmăţui and Galati 56 km. In each village, the samples were collected from 6 points. Typical sources analysed were: piped water, open dug wells, boreholes with a hand pump, surface water. Water quality data were analyzed during 2015-2016.

Fifteen physical and chemical parameters were studied. Some of the parameters were: density, turbidity, temperature, dissolved oxygen, biochemical oxygen demand, pH, resistivity, electrical conductivity, the density of the conductivity, salinity, total dissolved solids, nitrate nitrogen and ammonical nitrogen, sodium and potassium. The quality of the samples were analysed in order to identify the contamination problems. The water pollution status were evaluated according to the standards suggested by WHO (*Guidelines for Drinking-Water Quality*, 4th ed.; World Health Organisation: Geneva, Switzerland, 2012).

NPK analysis of the thermal degradation of selected brominated flame retardants

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Given the relatively low volatility of some brominated flame retardants (FRs), high elution temperatures are needed when applying chromatographic techniques for investigating their presence in matrices related to human exposure to these compounds, such as indoor dust samples or food items. Therefore, FRs might undergo thermal degradation, affecting analysis results, but no systematic study has been reported, while only a few papers report basic thermal degradation data for polybrominated diphenyl ethers (PBDEs).

We have investigated the thermal degradation of decabrominated diphenyl ether (BDE 209), a FR which accounts for more than 90% of the total PBDEs reported from indoor dust samples from Eastern Romania, by simultaneous TG/DTA coupled with EGA-FTIR/MS under various conditions. Kinetic analysis of non-isothermal data was performed by NPK method, and the information obtained by investigation of the computed isothermal and isoconversional vectors, in correlation with EGA information on the degradation products and molecular modeling results, provided valuable insight into the kinetics and mechanism of BDE 209 thermal degradation. The conclusions were aimed at designing proper specific GC analytical methods for the selected FRs and serving for a better estimation of the human exposure to such compounds.

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Mitoxantrone - surfactants interaction: a physicochemical overview

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As the cell membrane is the first barrier encountered by drugs and as surfactant micelles are known as model systems for biological membranes, the drugs-surfactants interaction has been the subject of great interest. Further, the general understanding of the drug-biomimicking structures interaction may provide helpful information for the design of potential delivery systems in order to control the physicochemical properties and bioactivities of encapsulated drugs.

The present work describes the physicochemical aspects of the interactions between anticancer drug mitoxantrone and anionic, cationic and non-ionic surfactants. Mitoxantrone-micelles binding constant, partition coefficient of drug between aqueous and micellar phases and the corresponding Gibbs free energy for the above processes, and the probable location of drug molecule in the micelles are discussed.

The disaggregation efficiency and the biocompatibility of these surfactants make them an attractive choice for potential delivery systems for mitoxantrone.

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Dopamine effects on self-assembled monolayers of L-cysteine on GaAs (100) electrodes

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Dopamine is one of the most significant catecholamines known to play a very important role as neurotransmitter. Lower concentration of dopamine may cause neurodegenerative diseases such as Parkinson and Alzheimer.

The effects of dopamine on L-cysteine modified p- and n-GaAs(100) electrodes have been investigated by electrochemical impedance spectroscopy (EIS) coupled with photoelectron X-ray spectroscopy (XPS) and atomic force microscopy (AFM).

EIS investigations indicate that dopant nature plays a key role in the dopamine interaction with L-cysteine modified GaAs(100) electrodes. For n-GaAs(100) electrodes, the presence of dopamine modifies the potential dependence of the main capacitive and resistive contributions controlling the electrode/solution interface, whereas for p-GaAs(100) this effect is not observed. The new species appeared in the N-1s and S-2p spectral regions indicate the interaction of dopamine with L-cysteine thiolate self-assembled monolayers at both p- and n- GaAs(100) electrodes. Although these species disappear under the electrochemical bias, dopamine does not leave the n-doped electrode surface and disturbs its electrochemical behaviour.

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Interaction between new mononuclear lanthanide(III) complexes of symmetrical tripodal ligands and *Saccharomyces cerevisiae* cells

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Lanthanide(III) ions have no intrinsic biologic significance, but they exhibit a high affinity for Ca²⁺ sites of proteins arising from similar ionic radii, but superior charge and coordination number with respect to calcium(II). Hence, they can either stimulate or inhibit the calcium-targeting native enzyme based on the initial role of the genuine metal ion: structural and catalytic, respectively [1].

Following a brief description of an original study regarding the correlation between Ln³⁺ accumulation, their toxicity and their potential to block the exogenous stress-induced Ca²⁺ influx into the cytosol of yeast cells [2], a structural characterization of LnL-type complexes (H₃L = Schiff bases derived from tris(2-aminoethyl)-amine and 3,5-disubstituted-salicylaldehydes) by the means of SC-XRD, NMR, and TGA is presented. The results of a chemogenomic screen for LnL sensitivity are explained starting from the ligand versatility in binding metal ions.

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Design, modelling and optimization of a MEMS gas sensors

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The paper presents the optimization of a heated gas sensor, by means of modelling and Finite Elements Analyses (FEA). The microsensor is patterned on both sides: the miniaturized IDT (interdigitated transducer) electrodes made on Ti(50nm)/Au(150nm), patterned on the front side of the wafer and a Ti/Pt micro-heater patterned on the back side of the wafer. The main purpose was to quickly and efficiently optimize the micro-heater according to the required application needs, in terms of maximum temperature, geometrical temperature distribution, time to heat the substrate and power consumption.

Several design iterations and different substrate types (ceramic and silicon) were analysed. In the final version, working temperatures between 250°-700°C can be reached by applying 5-15V for 5-30 sec.

Design and technology of micromachined gas sensors

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The research proposes to design and to develop the micromachining based technology for gas sensors used to monitor pollutant and explosive gases. The optimized metal oxides based gas sensors for monitoring very low concentration of pollutant and explosive gases to be used in houses, or industrial places will be presented. The design, sensors fabrication and testing results will be provided. Several chemical sensors based on nanostructured metal oxides (SnO₂:ZnO, SnO₂, ZnO, SnO₂:ZnO:Fe₂O₃) have been fabricated and tested for CO, C₃H₈ and CH₄ detection. Miniaturized IDT (interdigitated transducer) electrodes made on Ti(50nm)/Au(150nm), patterned on front side of a 0.2mm thick alumina wafer and deposited with different nanostructured metal oxides together with a Ti/Pt heater patterned on the back side of the alumina wafer have been fabricated. Working temperatures between 250°-550°C can be reached by applying 15V for 5-20 sec.

Physicochemical characterization of inclusion complexes formed by captopril and beta-cyclodextrin

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Captopril, an angiotensin I-converting enzyme inhibitor widely used for the treatment of hypertension, is a suitable candidate to be formulated in sublingual tablets, the best emergency pharmaceutical form to be used by the patient himself. In order to provide this drug in a more accessible and patient compliant form, its bitter taste must be masked and the best way to do this is the inclusion of captopril in beta-cyclodextrin cavity. Cyclodextrins are cyclic oligosaccharides that have a hydrophilic character at the external surface and a lipophilic one at the internal cavity level. CDs act as host molecules to form inclusion complexes with a wide variety of guest molecules.

Herein we investigate the ability of β-CD to include captopril. In order to obtain the inclusion complexes of captopril with β-CD we used the pasta method of complexation in solid state, and to compare the results of characterisation tests of the complex we prepared simple physical mixture. The study includes the physicochemical characterization of the inclusion complex by Fourier transform – infrared spectroscopy, X-ray diffraction, scanning electron microscopy and simultaneous thermal analysis. By all studied tests, it is obviously that captopril forms stable complexes with β-CD in 1:2 molar ratio, and the complexation was almost complete.

Thermal behaviour of some M^{2+} – hydrothermal carbon composites

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Hydrothermal carbons (HC) obtained via the hydrothermal carbonization of the individual carbohydrates or complex biomass permit the synthesis of semi-carbonized functional carbon materials with important applications ranging from catalysis and adsorption to biomedical and energy-related one.

The present study is focused on the thermal behaviour of several HC materials functionalized with metal cations in order to scrutinize the possibility of using these materials as precursors for different metal oxide (air atmosphere processing) and metal oxide – carbon composites (inert atmosphere processing). Several variables were taken into account: (1) the nature of carbohydrate (dextran, starch); (2) the nature of the metal cations (Co^{2+} , Zn^{2+}); (3) the ratio carbohydrate/metal cations; (4) the functionalization procedure (*in situ* or post-functionalization).

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Spectrophotometric studies of new chromenopyridines

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Nitrogen-containing heterocyclic building blocks are of great importance to both medical and organic chemists, and their synthesis continues to represent a challenge from both academic and industrial perspectives. Chromenopyridines derivatives are an important class of heterocyclic compounds, some of them exhibit significant biological activities, such as antibacterial, antitumor, antiasthmatic and hypotensive activities. As part of our current studies on the development of new routes to heterocyclic systems in under solvent-free conditions, we report here a new synthetic approaches under green conditions to several heterocyclic systems 4-amino-5H-chromeno[3,4-c]pyridin-5-one derived from enamincoumarine. Interesting fluorescent properties have been observed and studied for these new chromenopyridines. Thus, the influences of different internal and external factors (substituents and solvents) on the fluorescence of the synthesized products and also their selectivity and sensitivity against different metal ions were investigated by fluorescence and absorption spectroscopy.

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New substituted aminopyrazole with potential antitumor activity

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A series of novel substituted N-[(1H-pyrazol-1-yl)methyl]-3'-amino-1H-1,2,4-triazole were synthesized and characterized by IR, ¹H-NMR, ¹³C-NMR, UV-Vis.

We will be investigated the antitumor activity of the new pyrazolo-triazole derivatives.

La₂O₃ influence on physico-chemical properties of some silicate sealants for SOFCs

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Among various renewable sources, Solid Oxide Fuel Cells (SOFCs) represents a class of electrochemical devices which converts directly and efficiently energy produced by chemical reactions into electric power with low emission pollutants. Some glasses and glass-ceramics in the SiO₂-Al₂O₃-CaO-(Na₂O/K₂O)-La₂O₃ system are prepared and tested as seal candidates for solid oxide fuel cells (SOFCs). Structural, thermal and electrical characterization of raw and aged glasses at 850 °C for 100 h was attained by means of XRD, Raman spectroscopy, SEM, DSC, dilatometry and electrical conductivity measurements. X-ray diffraction and Raman spectroscopy were used to quantify the crystalline degree as well as the Qⁿ units (where n stands for bridging oxygen atoms of the SiO₄ units) in the vitreous phase of the as-prepared samples and their aged counterparts. Good thermal stability of all the obtained seals is pointed out by a higher ΔT=T_c-T_g difference than 200 °C (where T_g >700 °C). A slightly changed CTE values (9-11×10⁻⁶/K range within 200-700 °C) along with low electrical conductivity by aging is an indication of suitability of these materials for seals purposes.

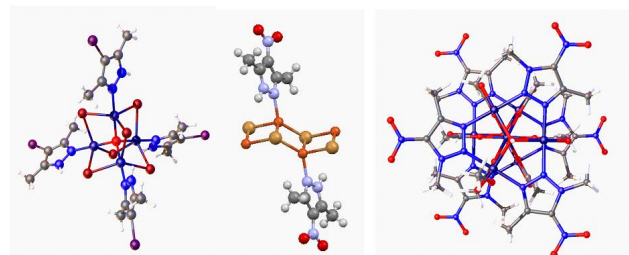
Structural variety of polynuclear copper complexes based on new pyrazoles derivatives

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We report the synthesis and structural analysis of some new polynuclear copper complexes based on 3,5-dimethyl-4-nitropyrazole and 3,5-dimethyl-4-iodopyrazole. Depending on pyrazole derivatives and the anion type we obtained a structural variety on copper polynuclear complexes.(Fig.1.) Compound **1** exhibit a (μ_4 -oxo)-tetranuclear structure formed with bromide bridging ligands and iodopyrazole derivatives as terminal ligands, since the compound **2** based on nitropyrazole derivatives shows a ladder type structure. Compound **3** is a heptanuclear complex with an astonishing structure, consisting two (μ_3 -oxo)-trinuclear units with nitropyrazole derivatives as



bridging ligands, connected through the acetate groups to a central copper ion. Spectral and magnetically measurements are discussed.

Figure 1. Synopsis of molecular structures for **1-3**.

The effect of soil burial degradation on cellulose fiber-filled polypropylene composites

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Protection of the environment lead to an increasing interest in the biodegradation of plastic materials considered as resistant to assimilation by microorganism. At the end of service life, enormous quantities of plastic wastes are disposed on landfill reducing water penetration and soil fertility. The biodegradation rate could be improved using composites based on biorenewable filler which facilitate the access for microbial communities from soil. In the present study, an outdoor soil burial test was carried out to evaluate the degradation in natural soil of several formulations of composites based on virgin and recycled polypropylene. The composition varies between 40-20% cellulose and 60-80% polyolefin polymer, respectively. The structural and morphological changes was analyzed by Fourier transform infra-red (FT-IR) and scanning electron microscopy (SEM). The results demonstrated that polyolefins based composites are subjected to a slowly process of biodegradation in soil.

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Cytotoxicity of *Sorbus domestica* L. extracts on animal and plant cells

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Sorbus domestica L (Rosaceae) is a spontaneous species cultivated in the past, spread throughout South Europe, Asia Minor and North Africa. Its fruits are edible, fresh or prepared. The bark may be used in the leather industry. In the traditional medicine it is used in intestinal diseases, diabetes and for memory improvement.

Within this work the results of toxicity tests on plant and animal organisms will be shown, for a hydro-alcoholic and aqueous extract obtained from *Sorbus domestica* L. leaves. The biological material, obtained from Gorj county was examined macroscopically and microscopically. The toxicity of the aqueous and hydro-alcoholic extracts (ethanol 50%) was assessed on plant (*Hordeum vulgare* L., on the range of 0.03-3.33%) and animal cells (lethality test on *Artemia franciscana* Kellog, on the range of 625-10,000 mg/L). The influence of the extracts on *Hordeum vulgare* L. seed germination has also been investigated. The polyphenolic content was established spectrophotometrically (Folin-Ciocalteu method). The results of the toxicity assays on plant cells showed that the aqueous extract did not affect root elongation significantly. The hydro-alcoholic extract inhibited root elongation strongly at concentrations higher than 1.66%. None of the two extracts affected germination and none was toxic on animal cells at the concentration ranges evaluated.

Evaluation of the Danube water quality near Galati City using WQI and multivariate analysis

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In this studies were used WQI and multivariate analysis to evaluate the quality of a surface water near Galati City. It was measured 12 parameters at 2 sites near Galati City, along the Danube River. The parameters that were analyzed between 2006 and 2013 are: T, pH, Rf₁₀₅, DO, COD, N-NH₄⁺, N-NO₂⁻, N-NO₃⁻, CN⁻, P total, Fe-total. The analysis was made in order to investigate spatiotemporal variations and to identify potential pollution sources. The samples were either analyzed on the field or sent to the laboratory for testing water (CREDENTIAL Center belonging to "Dunărea de Jos" University of Galati, Romania). Physico-chemical parameters analyze was determined according to Romanian and international standards in force.

WQI was calculated according to Weighted Arithmetic Water Quality Index Method and the identification of interdependencies between analyzed parameters was used to determined potential sources of pollution. So, it was applied statistical analyses based on identified correlations between the investigated parameters.

Eco-friendly synthesis and molecular modeling of some benzimidazole compoundsD.-G. Tudorache¹, M. Marinescu¹, G. Marton², C. Stavarache³ and C.-M. Zalaru¹¹University of Bucharest, Faculty of Chemistry, 90-92 Pandurilor, 010184, Bucharest, Romania²University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu, 011061, Bucharest, Romania³Institute of Organic Chemistry C.D. Nenițescu of the Romanian Academy, 202B Splaiul Independentei, 060023, Bucharest, Romania

Eco-friendly, one-pot, free-solvent synthesis of new benzimidazoles was performed. New N-Mannich bases were obtained from the synthesized benzimidazoles using the classical method. The structures of all compounds were confirmed by elemental analysis, ¹H-NMR, ¹³C-NMR and FTIR spectroscopies.

A density functional theory analysis of all molecular structures was performed and electronic parameters: chemical hardness, electronic chemical potential, global electrophilicity index were computed. Mullikan atomic charges and geometric parameters of the benzimidazole compounds were calculated with GAMESS [1]. It was found that the new N-substituents determine specific reactivity for each synthesized compound.

[1] R. Peverati and D. G. Truhlar, *J. Phys. Chem. Lett.*, 2 (2011) 2810-2825.

Bimetallic nanoparticles use as signal amplifiers for biosensors construction

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In developing sensitive and easy to use analytical tools the key-issues are raised by the main characteristics queries related to the signal sensitivity ensuring. In the case of sensors and biosensors this is decided by the analyst capability of designing the perfect match between appropriate transduction and biorecognition element functionality. Generally by using signal amplifiers, electrochemical sensors response in enhancing, normally nanoparticles/nanowires being widely utilized in this purpose. Pt@M bimetallic nanoparticles and Carbon Nanofibres-Gold Nanoparticles were used to increase the sensitivity of a biosensor for TCE/PCE contaminants analysis. As biorecognition element for TCE/OCE analysis the exploitation of PSII enriched membranes was considered appropriate for the development of electrochemical biosensors, as the biomediator is selectively activated by light, consequently minimizing the electrochemical interferences. Various photosynthetic strains were tested. The optimized biosensor (based on wild type strain) was further completely characterized. The results obtained using a new developed PSII-Pt@Au_CSPE amperometric biosensors applied in assessing the urban water contaminants proved a sensitivity of 15nA/μmolL⁻¹ for TCE/PCE contaminants.

Acknowledgements:

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**Polyol-assisted synthesis of zinc oxide spherical aggregates
with multifunctional properties**

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Zinc oxide (ZnO) is a multifunctional oxide-based material with an extraordinary technical potential due to a unique combination of properties, for example semiconducting, optical, piezoelectricity and pyroelectric peculiarities. Herein we report an additive-free polyol procedure that affords, in one-step and mild conditions, highly crystalline zinc oxide nanoparticles, aggregated in hollow and solid spherical shaped structures. The adjustment of the synthesis parameters (reaction time and temperature, zinc cation concentration, polyol types) tunes the size of ZnO crystallites, the size and the shape of the ZnO aggregates, as well as the surface characteristics and nature/concentration of the defects and, as a consequence, the luminescent properties. The structural, optical, photocatalytic and antimicrobial properties of the obtained ZnO products will be discussed.

SECTION 7

Catalysis and chemical engineering

KEYNOTES

On the kinetic of structure sensitive reactions over well-defined metal nanoparticles: lean reduction of NO with C₃H₆ and ammonia synthesisIoan Balint¹, Ken-ichi Aika² and Eugen Segal³¹Institute of Physical Chemistry of Romanian Academy "Ilie Murgulescu", Romania²Tokyo Institute of Technology, Japan³Professor Eugen Segal, University of Bucharest, 1933-2013

Use of well-defined metal nanoparticles allows the identification of kinetic data free of transport effects and thus, by applying Madon–Boudart criteria, the rigorous calculation of kinetic parameters is at hand. One of the chosen reaction with practical significance is lean reduction of NO with C₃H₆ over cubic Pt nanocrystals of ≈12 nm deposited on Al₂O₃. Another analyzed structure sensitive reaction is ammonia formation over uniform Ru nanoparticles of around 5 nm dispersed on acid (Al₂O₃) and on basic (MgO) supports. In contrast to conventional impregnated catalysts, the values of TOF (turnover frequency), in kinetic region, are little affected by metal loading and by nature of support due to minimal metal-support interaction.

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Solid-gas phase synthesis of ammonium paratungstate and amine-WO₃ hybrid catalystsD. Hunyadi¹, E. Majzik¹ and I. M. Szilágyi^{1,2}¹Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, H-1111 Budapest, Szt. Gellért tér 4. Hungary²MTA-BME Technical Analytical Chemistry Research Group, H-1111 Budapest, Szt. Gellért tér 4. Hungary

From ammonium paratungstate (APT), (NH₄)₁₀[H₂W₁₂O₄₂]·4H₂O tungsten oxides, tungsten carbides or tungsten metal can be prepared, all of which are significant for various industries (catalysts, photocatalysts, gas sensors, cutting and drilling tools, lighting industry). Thus, on the one hand, in this study the reaction between WO₃ powder, NH₃ and H₂O vapors was investigated with the aim of preparing APT. The effects of the composition, crystal structure and particle size of the WO₃ powder were investigated along with the effect of the partial pressure of ammonia and water vapor on the products. The results indicated that the properties of the as-prepared APT were identical to the commercial APT material. In addition APT nanoparticles were produced for the first time. On the other hand, the solid-gas phase reaction between tungsten oxide powder, ethylene-diamine and water vapors was also investigated with the goal of preparing amine-WO₃ hybrid materials, which can be used in water purification, catalysis and absorption. In addition, we also prepared these hybrids by crystallization from aqueous solutions. The two methods yielded the same product, the only difference was in the morphology. All reactions were monitored and the products were characterized by powder X-ray diffraction (XRD), Fourier transformed infrared spectroscopy (FTIR), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and thermal analysis (TG/DTA-MS). Furthermore, the catalytic activity of selected samples was tested in a model reaction.

Understanding the effect of surface phosphorus on the enhanced selectivity of NiO in ethane oxydehydrogenation by using *in situ* electrical conductivity measurements

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In situ electrical conductivity measurements (ECM) constitute a powerful technique for the investigation of electronic and redox properties of oxidation catalysts and, therefore, can help understanding their catalytic behavior [1]. The effect of adding P to the NiO surface on its catalytic performance in the low-temperature ethane oxydehydrogenation (ODH) was investigated and the role of surface P was unambiguously explained by *in situ* ECM. Thus, surface-phosphated NiO catalysts with different P contents were prepared and tested in ethane ODH in the temperature range from 300 to 425 °C. Their electrical conductivity was studied as a function of temperature and oxygen partial pressure and was followed with time during sequential exposures to air, ethane–air mixture (reaction mixture) and pure ethane in conditions similar to those of catalysis. By adding increasing amounts of P to NiO both the concentration and mobility of the surface lattice O⁻ species in the NiO decrease considerably and, therefore, its catalytic selectivity in ethane ODH is strongly enhanced.

S. B. Ivan thanks UEFISCDI for the Young Researcher Fellowship awarded under the contract no. 5/05.01.2015.

[1] J. M. Herrmann, in: *Catalyst Characterization, Physical Techniques for Solid Materials*, B. Imelik and J. C. Védrine (eds.), Plenum Press, New York, 1994, ch. 20.

Photocatalytic properties of ALD coated polymer and inorganic nanostructures

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Crystalline titanium-dioxide is a widely used photocatalyst, but amorphous TiO₂ is considered not to have photocatalytic activity. Recently it has been found that amorphous TiO₂ deposited by atomic layer deposition (ALD) might have photocatalytic activity. During our work we studied the properties of ALD grown amorphous and crystalline TiO₂ and as a reference, we examined ALD Al₂O₃ and ZnO. The oxide layers were deposited on SiO₂ and PMMA (poly(methyl-methacrylate)) nanoparticles, PVA (poly(vinylalcohol)) and PVP (poly(vinylpyrrolidone)) nanofibers. The bare and core/shell composite nanoparticles and nanofibers were investigated by SEM-EDX, TEM, FT-IR and XRD. Finally, the photocatalytic activities were studied. The photocatalytic reactions were investigated by the decomposition of aqueous methylene orange, monitored by UV-Vis. The TiO₂ prepared at 50 and 80 °C was amorphous, while at 300 °C it was crystalline, the Al₂O₃ was amorphous at 50 °C, 80 °C and 250 °C and the ZnO was crystalline at all temperatures. The amorphous TiO₂ deposited on the SiO₂ and PMMA nanoparticles indeed had some photocatalytic effect, the Al₂O₃ was not active, while the ZnO showed good photocatalytic activity. The photocatalytic performance was greatly influenced by the type of the support material.

**Photocatalytic removal of trichloroethylene (TCE)
over Au/TiO₂ and Pd-Au/TiO₂ using solar simulated radiation**

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The photocatalytic removal of TCE pollutant in aqueous solutions under simulated solar irradiation (AM 1.5) is investigated. One of the greatest practical impediments for practical application of conventional catalytic hydrodechlorination (HDC) reaction in dark condition is that H₂ reductant must be introduced in reacting system. The advantage of photocatalytic method is that ·OH radicals generated under light irradiation are able to mineralize the organic pollutant to CO₂ and Cl⁻ (HCl). The photocatalysts, Au and Pd-Au supported on TiO₂, were synthesized by impregnation and deposition-precipitation methods. The research explored two ways for TCE abatement: by photomineralization and by combined photomineralization/ HDC reaction. In the second case, small amount of CH₃OH was added to the reacting system to promote the formation in situ of solar H₂. Thus, fraction of TCE was converted to Cl⁻, ethane and ethylene using as reductant the photocatalytically produced H₂. The Au/TiO₂ showed higher activity for photomineralization of TCE compared to simple TiO₂ whereas Pd-Au/TiO₂ were more efficient to catalyze the TCE removal by combined photomineralization/HDC reaction.

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SECTION 7

Catalysis and chemical engineering

POSTERS

Morphology-dependent photocatalytic and antimicrobial activity of SiO₂ and SiO₂-TiO₂ composites

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Unusual physical and chemical properties coming from the highly defected SiO₂ and from the derived composite materials are investigated. SiO₂-TiO₂ composites are widely used and studied due to the wide range of applications. Recently, the biocompatibility/bioactivity was put in evidence. The sol-gel preparation-protocol involved the following steps: the sol and gel formation by hydrolysis of precursor, ageing of gel for 3 hours, filtering, drying and thermal treatment at 500 °C for 3h. The X-ray diffraction of composites evidenced only the amorphous SiO₂, due to the tiny quantity of TiO₂ (smaller than 1%). The SEM, XRD AFM, FT-IR, UV-VIS, XPS and BET analyses were also performed in order to identify a correlation between the structural and optical characteristics and their photocatalytic/antibacterial properties. The experimental results confirmed that the structural characteristics of SiO₂-TiO₂ are strongly interrelated with light absorption/antimicrobial activity. The bactericidal/bacteriostatic effect of TiO₂-SiO₂ was evidenced for both Gram positive and Gram negative bacteria.

Selective reduction of nitrate from water using Pd-Cu catalysts supported on anion exchange resins

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Water pollution with nitrates and nitrites becomes a major problem worldwide. Liquid-phase catalytic nitrate reduction, first time reported in 1989 by Varlop, seems to be a convenient technique for the removal of these pollutants from natural water. Besides the active phase, the nature of the support has shown to affect the catalyst performances. In this work, a series of bimetallic Pd-Cu catalysts (with 2% Pd and 0.5% Cu) supported on various anion exchange resins (A-520E, A-500P and A-501P from *Purolite*) was prepared by different techniques. There are two reasons in choosing the resin as supports: (i) to ensure a high dispersion and controlled distribution of the active components; (ii) to enable the NO₃⁻ internal diffusion. For the assessment of the catalyst stability, the leaching of Cu and Pd in the treated water were quantified by AAS. It was found that the activity and selectivity of the catalysts strongly depend on the method used for the deposition of the second metal (ion exchange or controlled surface reaction), but also on the support characteristics, such porosity and ion exchange capacity.

CO oxidation on Pd/TiO₂ and Pd/SnO₂/TiO₂

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The oxidation reactions of CO on Pd/TiO₂ and Pd/SnO₂/TiO₂ catalysts were studied for their possible use in environmental problems. The samples were prepared by the impregnation method. The structural and textural properties of the obtained powders have been characterized using BET, XRD and SEM. Their redox properties were tested by using TPR technique and the surface dynamics was studied by electrical conductivity measurements in similar conditions with those encountered in the practical use in catalysis.

The catalyst samples were tested in the catalytic oxidation of CO in the 30-400°C range of temperature. It was found almost a total conversion above 200°C for both samples. The physico-chemical properties of samples and their performances in CO oxidation reactions were correlated in order to detect the nature of the active sites.

Enhanced photocatalytic activity of ZnO nanoparticles obtained by “green” synthesis with well dispersed Pd-Au bimetallic nanoparticles

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ZnO nanostructured materials are promising photocatalysts because of their non toxicity, low cost and good stability. Noble metals (Au, Ag, Pd) supported by ZnO have attracted significant interest, as it may possibly result in a superior catalyst with enhanced photocatalytic activity.

The ZnO nanoparticles were obtained using the extract of black tea solid waste and Zn acetate dehydrate in alkaline medium. Bimetallic nanoparticles. of around 10 nm were obtained in a so called “green” way by simply adding a solution containing the gold precursor (HAuCl₄) and palladium precursor Pd(NO₃)₂ in a tannic acid solution. The surface and chemical state analysis of pure ZnO and Pd-Au decorated ZnO were investigated by XRD, SEM-EDX, TEM, IR-spectroscopy, CO chemisorptions and UV-Vis spectroscopy. The photocatalytic activities were evaluated by nitrate reduction reactions in aqueous solutions. The Hg lamp of 150 W was used as a source for photocatalytic study. Compared with ZnO nanoparticles, Pd-Au loaded (2%) on ZnO catalyst presented increased activity, which has been evaluated in terms N₂ selectivity.

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Complete oxidation of aromatic hydrocarbons on Cu-Mn mixed oxides catalysts

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Alumina supported Cu-Mn oxide catalysts were prepared using Mn and Cu acetates as precursors. The samples were characterized with BET method, magnetic susceptibility, XRD, XPS, TPR and TPD. The use of formates as precursors and their decomposition without preliminary melting is especially important for the synthesis of supported oxide catalysts. The formation of the catalytically active oxide phase in this case is a complex process because it is affected by both the presence of a "chromatographic effect" and the crystallization in the pores of the support. The red-ox process $\text{Cu}^{2+} + \text{Mn}^{3+} = \text{Cu}^+ + \text{Mn}^{4+}$ plays very important role with respect to the formation of the Cu-Mn compound having a spinel type structure. At low temperatures the equilibrium is shifted to the left while with increasing the temperature a shift to the right is predominating, hence it favors the appearance of Cu^+ . The metal ions change their coordination, as a result of which Cu^+ is formed with an enhanced Mn^{4+} content. The catalysts exhibited catalytic activity in the complete oxidation of benzene, toluene, ethylbenzene and izoprophylbenzene.

Electrical properties and gas sensor performance for Zinc-Titanium-Iron mixed oxides

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In situ Impedance Spectroscopy measurements of a series of ZnTiFe mixed oxides materials was performed in the range of 100Hz-5MHz at different temperature (200-400°C) in air and target gas (CO), in order to evaluate the influence of the components (Zn, Ti, Fe) on electrical conductivity of the surface/intergrain contact. The sensing performance for CO detection of the prepared powders have been tested in the range of 100-1000 ppm.

Effect of monometallic (Au and Pd) and bimetallic (Pd-Au) loading on the complete oxidation activity of Y-doped ceria catalysts

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The detoxification of volatile organic compounds (VOCs) remains one of the global environmental problems. The aim of the present study was to examine the effect of different methods for Y-modification of ceria on the structural, reductive and catalytic properties of mono Au, Pd and bimetallic catalysts (Pd loading over already deposited Au particles) in complete benzene oxidation (CBO) and complete propene oxidation (CPO). Three series of Au (3 wt.%), Pd (1 wt.%) and Pd-Au (1 wt.%)–Au (3 wt.%) catalysts were synthesized using as supports ceria, Y-doped ceria prepared by impregnation (IM) and Y-doped ceria prepared by co-precipitation (CP). The dopant amount was 1 wt.% Y₂O₃. The catalysts were characterized by XRD, XPS and TPR. The Pd catalysts demonstrated higher oxidation activity as compared to the corresponding Au catalysts in CBO and CPO. The best performance in both reactions exhibited the Pd-Au catalysts. The highest activity and good stability was established over Pd-Au catalyst on Y-doped ceria support prepared by IM. The results of 100% propene total oxidation at 180 °C and especially the benzene combustion at temperature as low as 150 °C make this Pd-Au catalyst promising for practical application aiming VOCs abatement.

Heterogeneous activation of Oxone using cobalt phthalocyanine-supported reduced graphene oxide: Application for rhodamine B degradation

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Rhodamine B (RhB), a cationic xanthene dye used in textile, printing, and photographic industries presents carcinogenicity, neurotoxicity, and chronic toxicity towards humans and animals [1]. Thus, RhB elimination from wastewater effluents is a subject of considerable concern of environmental remediation. In the present work, a cobalt phthalocyanine-supported reduced graphene oxide material (rGO-CoPc) was used as a catalyst for the RhB degradation in the presence of peroxymonosulfate (Oxone). The catalytic activity of the rGO1-CoPc1 catalyst (rGO:CoPc = 1:1) was evaluated by UV-vis absorption spectroscopy at different Oxone concentrations and rGO1-CoPc1 dosages. The apparent reaction rate constant presents a non uniform variation with both the catalyst dosage and Oxone concentration. The catalytic mechanism of Oxone activation on rGO1-CoPc1 composite is explained by heterogeneous reactions analogous to those proposed for heterogeneous Fenton-like reaction. The removal efficiency is observed to be as high as 100% during 11 cycles, suggesting a long-lasting catalytic activity of the of rGO1-CoPc1/Oxone system.

Reference:

[1] H.-J. Cui, H.-Z. Huang, B. Yuan, M.-L. Fu, *Geochem. Trans.* 16 (2015) 10.

**Photocatalytic degradation of Brilliant Blue dye in aqueous phase
by supported titanium on KIT6 mesoporous silica.
Effects of reaction pH and synthesis method on kinetics and mechanism**

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Brilliant Blue dye is a food coloring approved in the EU and USA and a pharmacologically inactive substance for manufacturing drugs. In this paper we report the photocatalytic degradation of Brilliant Blue in the presence of Ti-KIT6 nanoparticles. The photocatalysts were synthesized by two methods: direct synthesis and impregnation. In both synthesis the surfactant was P123, cosurfactant was butanol and pH acid. The obtained materials were characterized by N₂ adsorption-desorption, SEM microscopy, X-ray diffraction and UV-Vis spectroscopy. These results evidenced the preservation of KIT6 mesoporous ordered structure after titanium immobilization. A low effect of metal incorporation on surface area, porosity and pore size was evidenced for both Ti-KIT6 materials. The photocatalytic properties were tested in condition of UV-light irradiation (254 nm) and aqueous solution. The reactions were carried out at room temperature in acid, neutral and alkaline pH conditions. The best results were obtained in acid pH conditions of the photocatalytic reactions. This confirmed the presence of the positive holes (TiOH₂⁺) on catalyst surface, that are considered as the major oxidation species at low pH of photocatalytic reactions, as well the increasing of azo dyes degradation rate for lower pH.

**Support effect of nano dispersed Rh-Cu bimetallic catalyst
on catalytic denitration for water cleaning**

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The problem of nitrate contamination in groundwater and surface water is of great concern. A big source of nitrate contamination in the environment is industrial waste, landfill leachate, agriculture runoff and human disposal.

The aim of this work was to study the effect of nano dispersed Rh-Cu bimetallic catalysts supported by TiO₂, WO₃, CeO₂ and Al₂O₃ on liquid phase nitrate reduction. The Rh-Cu bimetallic nanoparticles were synthesized by polyol alkaline method and then characterized by XRD, XPS, TEM and fractal analysis. The catalysts obtained by impregnating various substrates with Rh-Cu nanoparticles were characterized by XPS, BET surface area, TPR and hydrogen chemisorptions.

The Rh-Cu nanoparticles supported by TiO₂, WO₃, CeO₂ and Al₂O₃ (1 % metal loading) showed excellent activity for catalytic reduction of NO₃⁻ ions in water phase.

The nanoparticle-based catalysts, synthesized in a controlled morphology and dispersed on various support materials are very promising candidates for practical applications such as water cleaning.

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Solid-state reaction of Ta-based perovskite and its photocatalytic performance in the degradation of trichloroethylene

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Among various materials, tantalum-based perovskites have received significant attention due to their superior photocatalytic properties. Alkali tantalates are good photocatalysts not only for splitting of water but also for the degradation of environmental pollutants. In this study, we report on the preparation of $\text{RbLaTa}_2\text{O}_7$ perovskite synthesized via a conventional solid-state reaction at different temperatures. The catalytic performance of perovskites was evaluated in the photocatalytic degradation of trichloroethylene (TCE) using a Xe short arc lamp of 150 W. Phase formation and physico-chemical properties of the as-prepared samples were studied in details by XRD, SEM, BET surface area, UV-vis and FTIR spectroscopy. It was revealed that the synthesis conditions (i.e. temperature, reaction time) highly affect the phase composition of rubidium tantalum oxide. $\text{RbLaTa}_2\text{O}_7$ perovskite exhibits intense absorption of UV light at a wavelength of about 250 nm. The conversion of trichloroethylene was dependent with the preparation conditions of the studied tantalum perovskite.

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Kinetics study of graphene-assisted hydrogen storage and scavenging

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Solid-state hydrogen storage is a major challenge in energy-related applications. It requires a high-gravimetric capacity acceptor operated at relatively low temperatures and fast absorption-desorption kinetics. Magnesium is a potent candidate for hydrogen storage, however, its slow hydrogen absorption/desorption kinetics, taking place only at high temperatures, prevents its practical application in hydrogen storage.

Improved kinetics have been achieved in composites consisting of transition-metal-based catalysts, nanocarbons and Mg. Gas-solid catalytic hydrogenation is a multistage reaction involving hydrogen atom spillover, from the catalyst to the carbon and then to the acceptor, followed by nucleation and growth of metal hydride. We previously showed that Pd-decorated CNTs, as hydrogen spillover agents loaded in Mg powder, accelerate hydrogen absorption/desorption kinetics by more than one order of magnitude. In this study the influence of graphene additive will be discussed in the terms of the hydrogen absorption/desorption kinetics.

**Photocatalytic degradation of trichloroethylene
on nanostructured Pt/TiO₂ catalysts: effect of thermoresponsive polymers**

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Photocatalytic degradation of trichloroethylene (TCE) was used as a test reaction to study the catalytic activity of nanostructured Pt supported on TiO₂. The Pt/TiO₂ catalysts were synthesized in the presence of new thermosensitive capping polymers, as structure directing agents, in aqueous medium and at room temperature. Catalysts characterizations were performed by TEM, Fractal analysis, XPS, XRD, CO chemisorption and UV/Vis spectroscopy techniques. The influence of temperature-sensitive polymers, consisting in a central block of polyethyleneglycol (PEG) and lateral blocks of statistical copolymers of N-isopropylacrylamide (NIPA) and N-t-butylacrylamide (TB), on the morphology and size of the Pt nanoparticles and therefore on the catalytic properties of Pt/TiO₂ catalysts was evaluated. The activity of nanostructured platinum catalysts (Pt–NIPA-TB-PEG/TiO₂) was compared with that of a Pt–PVP/TiO₂ catalyst. The efficiency of the Pt/TiO₂ catalysts depends on many factors that could be strongly affected by the structural and electronic properties of the material that depend on particle size and preparation method.

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SECTION 8

Sol-gel science and applications

KEYNOTES

Thin film SnO₂-ZnO composite metal-oxide semiconductor sensors for selective CO detection

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A series of bi-component SnO₂-ZnO metal oxide thin films were deposited on a home-made miniaturized transducer with a gold inter-digital electrode and a Pt heater.

The sensors with different SnO₂:ZnO ratios were prepared by sol-gel / dip-coating, a low cost technology.

Different gases (CO, CH₄, C₃H₈) were tested on a home made experimental setup, in various concentrations (200-1000 ppm). The gas sensing measurements (sensor sensitivity, response time, selectivity and recovery) were performed in environmental conditions (carrier gas is air) at different working temperatures (130-300⁰C). The gas-sensing behavior of the films was correlated with the structural, chemical and morphological properties of the multilayered structures.

It was found that the sensor sensitivity is less dependent on the film thickness but is significantly influenced by the SnO₂/ZnO ratio at the working temperature.

Sensor response, recovery, temperature dependence and the influence of humidity are reported.

Solid oxides with fluorite and apatite structures for SOFC electrolyte

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Nowadays, the research in the field of solid oxide fuel cells (SOFCs) is focused towards the decrease of operating temperature down to 700⁰C. In this study, ceria-based fluorite oxides and lanthanum silicate apatites have been synthesized using a Pechini modified method. The crystalline structures of calcined powders and sintered pellets were investigated using X-ray diffraction (XRD). The evolution of lattice parameter with dopant type and concentration was evidenced. Besides XRD, Raman spectroscopy was used for the identification of crystalline phases in the samples. The pellet morphology and the distribution of elements in the sinters were evidenced by SEM/EDS. The electrical conductivity was measured by electrochemical impedance spectroscopy using gold as electrodes. Measurements were performed under air, in the temperature range 200-800⁰C. The influence of dopants on the electrical conductivity of fluorites and apatites was shown.

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Structural, morphological, chemical and optical properties of TiO₂ sol-gel films doped with Nb and V

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TiO₂ films deposited on glass and Si substrates by the sol-gel - dipping method were studied, focusing on the influence of Niobium/Vanadium doping on the structure, surface chemistry and their optical and electrical properties. The TiO₂ films doped with 1.2 at. % Nb(V) crystallized in anatase phase as evidenced by XRD analysis. It was found that thicker films are obtained in the case of V-doped TiO₂ films, while the values of the optical band-gap show similar values. Bands related to the vibration of oxygen in the Ti-O, Nb-O and V-O bonds were identified based on Infrared Spectroscopic Ellipsometry, proving the incorporation of the dopants in the matrix of the TiO₂ films. Both types of doped films exhibit around 80 % transparency on a wide spectral range (300-1700 nm). Niobium and Vanadium have been identified in the surface / subsurface region in the 5+ oxidation state. From a morphological point of view, all titania films show a very uniform and compact microstructure, with a homogeneous superficial structure of small grains with diameters in the range of 10-20 nm.

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Lead-free ferroelectric alkali niobate based thin films: Solution synthesis – Microstructure - Properties relation

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Due to environmental concerns much of the current research has been oriented towards lead-free ferro- and piezoelectric materials. Potassium sodium niobate, K_{0.5}Na_{0.5}NbO₃ (KNN) and KNN-based solid solutions have been studied as potential replacements for lead-based piezoelectrics, both in bulk and thin film forms. Problems related to processing of alkali niobates are connected to the assumed deficiency of alkalines due to volatilisation, which hinders control over the stoichiometry, contributes to formation of secondary phases and deterioration of the microstructure. The problem can be overcome by adding alkalis in excess and/or by a partial substitution of the A- and/or B- site atoms. In the contribution we discuss the influence of the alkali excess in the coating solutions, chemical modification, and the annealing conditions on the crystallization and microstructure of thin films. We show how the film microstructure influences the dielectric, ferroelectric and local piezoelectric response of the films.

Fabrication of arsenic sulfide layers from solutions using arsenic sulfide dissolved in n-propylamine or prepared from arsenic trichloride and thiourea

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In last ten years chalcogenide layers have been investigated for photonic applications in the mid-IR spectral region such as passive and active waveguides, gratings, optical memories. A number of such applications is based on arsenic sulfide layers which are prepared by physical methods and from solution. In solution-based methods As_2S_3 layers are usually applied from solutions of arsenic sulphide in amines. In this paper the performance of two solution-based methods, one employing As_2S_3 in n-propylamine (PA) and second based on As_2S_3 prepared from arsenic trichloride and thiourea, for preparing layers of arsenic sulphide is discussed.

Two types of As_2S_3 solutions have been tested. One was obtained by dissolving of fine As_2S_3 powders in propylamine in concentrations from 0.3 to 0.6 mol/l. Second solution was obtained from AsCl_3 added into a solution of thiourea in PA. Solutions were applied by the dip-coating technique and applied layers were heat treated at temperatures up to 200 °C. Applied layers were characterized by optical microscopy, and by measuring their transmission and reflection spectra. Using measured spectra and theoretical models such as Swanepoel's one, refractive indices, thicknesses and As_2S_3 bandgaps were estimated. Layers with thicknesses up to 1500 nm and a maximum refractive index of about 2.2 have been fabricated by using solutions of As_2S_3 in n-propylamine. Obtained results and their relationship to the preparation approach used are discussed in the paper.

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Molecular strategies toward original nanomaterials at the frontier between soft chemistry and solid state chemistry

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Reactions between molecule-scale species are highly suitable for cost effective fabrication of materials with controlled crystal structure, nano-, meso- and micro-structures. Although such chemical pathways are intensively studied since three decades for nanostructured metals, chalcogenides and simple metal oxides, other compounds families were only scarcely, if ever, reported at the nanoscale. These systems show at the bulk scale mechanical, catalytic, optical and electronic properties without equivalent among common compounds. The design of corresponding nanostructures could then yield important changes or enhancement of existing properties, emergence of new behaviours and novel processing possibilities. This presentation will highlight some recent research efforts aiming at the design of functional nanomaterials with innovative elemental compositions, some of them being considered as “exotic” to chemist. We will discuss several cases showing properties different than those of bulk phases, including metal-boron alloys for thermoelectricity, multicationic oxides for fuel cells and boron-carbon-nitrogen frameworks for environmental remediation.¹⁻²

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Electrical characterisation of sol-gel multilayered TiO₂ films doped with transition metals

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We present results on the studies of TiO₂ multilayers deposited on Si substrates by the sol-gel method, focusing on the influence of Niobium/Vanadium doping on the electrical characteristics of MIS structures with incorporated doped TiO₂ films. Electrical measurements of the current-voltage and capacitance-voltage characteristics of MIS structures have pointed out that the doping level in the TiO₂:Nb(V) films should be equal or greater than 10¹⁶ cm⁻³. The character of current-voltage dependences and decrease of the specific resistivity ($\rho \sim 10^4$ -10⁵ Ωcm) by increasing the electrical field evidence for bulk character of electrical conduction in these TiO₂:Nb(V) films and reveal that the current through the films is space charge limited current via deep levels with energy distribution in the energy gap of TiO₂. The strong frequency dependence of the impedance characteristics of the MIS structures indicate that both capacitance and conductance are also frequency dependent, which in turn is evidence of the capture and emission of electrons at deep levels in the sol-gel TiO₂ energy band gap.

Mn doped ZnO thin films for harvesting applications obtained by sol-gel method

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Zinc oxide has recently been studied extensively due to its properties, that makes it suitable for many applications such as transparent electrode for solar cell, flat panel devices, organic light emitting diode (OLED), thin film transistor-liquid crystal display (TFT-LCD), gas sensors and harvesting applications. Sol-gel processes give the ability to produce films in a simple, low cost and highly controlled way. To improve its piezoelectric properties ZnO can be doped with different materials, such as Mn. In the present work we study thin films of Mn-doped ZnO with different doping concentration (0, 1, 2, 5 at %) that were deposited on Pt/TiO₂/SiO₂/Si substrates by dip coating method. We used two different consolidation methods for the deposited layers and the properties of the obtained films were compared. The structural, morphological and optical characteristics of the films were investigated by X-Ray Diffraction, Scanning Electron Microscopy, Spectroellipsometry, Atomic Force Microscopy, XPS spectroscopy and Electrical measurements. The obtained Mn doped ZnO films present interest in harvesting applications.

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Contribution to the chemistry of sol-gel and microwaved assisted sol-gel processes

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Among the non-conventional wet chemical processes of obtaining oxide nanostructures, the sol-gel method is one of the mostly used and studied as well. The most important step of the method is represented by the formation of the amorphous inorganic polymers in solution that allows properties tailoring of the resulted products. However, this first step is the most difficult to be investigated, due to the high number of reactions that take place simultaneously leading to formation of a high number of molecular species. In the presentation some information on the chemistry of the sol-gel processes, especially in the silica based systems, will be given based on gas chromatography coupled with mass spectrometry (GC-MS). The influence of microwaves (MW) on the sol-gel process in doped and undoped TiO₂ systems will be also discussed based on high pressure liquid chromatography (HPLC) investigations. Preparation and complex characterisation of oxide and hybrid nanostructures as films powders including 1D nanostructures), nanocomposites and some of their possible applications will be also presented.

SECTION 8

Sol-gel science and applications

POSTERS

**Doped TiO₂ gels and powders:
preparation, physico-chemical properties and solar-light photocatalytic activity**

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Gels and powders of Fe³⁺ doped TiO₂ were synthesized by sol gel process under alcoholic route by using titanium tetraisopropoxide and titanium ethoxide as titanium precursors. The prepared gels and powders have been thermally treated at 450°C for 1h, according to the Differential thermal and Thermogravimetric analysis. X-ray diffraction and Raman Spectroscopy have evidenced the TiO₂-anatase crystalline structure of the prepared samples. The morphology of the powders, consisting in nanometric anatase crystallites surrounded by amorphous areas has been investigated by high resolution Transmission Electron Microscopy images. The photo catalytic activity of Fe³⁺ doped TiO₂ gels and powders was proved using the photocatalytic mineralization of oxalic acid under simulated solar irradiation

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Properties of silica layers fabricated from silica sol containing silica nanoparticles

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Silica layers fabricated by the sol-gel method are usually amorphous and exhibit a relatively low refractive index ($n \sim 1.46$ at about $0.6 \mu\text{m}$), high optical transmittances from UV to near-IR ranges, and high thermal stability. They can be used as high reflection or antireflection coating, dielectric mirrors, bandpass filters, etc. However, crack-free layers with a thickness of about 400 nm can be prepared in one coating cycle from sols of simple alkoxides. This paper presents an approach for the preparation of silica crack-free layers with increased thicknesses using the dip-coatings technique and stable silica sols containing silica nanoparticles. Input silica sols were prepared from tetraethylorthosilicate (TEOS) with ethanol and HCl with concentrations 1-2 mol/l and RW 1.75. Silica nanoparticles were dispersed in water/TritonX-100 solution and added into some of the input sols. Both types of sols were deposited onto silica slides and silicon wafers by the dip-coating technique using different withdrawing velocities. Prepared gel layers were thermally treated at 450-900°C. The appearance and thickness of prepared silica layers were characterized by optical microscopy and scanning electron microscopy. Optical properties of layers were characterized by spectral ellipsometry and UV-VIS-NIR transmission and reflection spectrometry. The measurements have shown that characteristics of layers fabricated from both types of the sols differ and that one can obtain stable transparent silica layers with increased thicknesses from TEOS sols containing silica nanoparticles. This research was supported by the Czech Science Foundation (contract 16-10019S).

Iron doped TiO₂ films and nanopowders and their photoactivity in nitrobenzene removal from water

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In the environmental protection field TiO₂ holds one of the most important places due to its photocatalytic properties, both in the case of powders and coatings. The undoped and Fe-doped TiO₂ thin films deposited by spray pyrolysis method on glass substrates, at 373 K, and the sol-gel nanopowders with the same composition were prepared. The influence of Fe dopant concentration and of temperature of the thermal treatment on the obtained materials has been studied using: XRD, XPS, TEM and SEM techniques, and measurements of hydrophilicity properties and photocatalytic activity. For the samples that contain the lowest Fe content, the thermal treatment of the samples at 673 K lead to an increased super-hydrophilic performance and the best yield of nitrobenzene removal from water.

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Sol-gel doped TiO₂ nanopowders with photocatalytic activity - The influence of dopants on titania structure

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TiO₂ is well known as an excellent photocatalyst that permits the degradation and finally the mineralization of xenobiotic compounds from water. This paper highlights the effects of iron, cobalt and nickel dopants on the structure and photocatalytic properties of the sol-gel TiO₂ nanopowders and performs a comparative study of their behaviour. The dopants addition is responsible for supplementary defects in the crystalline lattice. The increase of temperature does not significantly influence the unit cell volume (UCV). This fact could be considered as a proof of the acceptance of the dopant by the anatase lattice, where Me_xTi_{1-x}O_{2-δ} type solid solutions are formed. The variation of the average size of crystallites (D) and the average lattice strains (S) values with temperature, calculated for both undoped and doped TiO₂ samples indicates the fact that the highest disorder state was found at 400°C. The photocatalytic activity of the prepared nanopowders has been tested in the degradation of nitrobenzene from water. The samples with 0.5 wt% Fe and 1 wt% Co and Ni dopant concentration thermally treated at 400°C presented the best photocatalytic activity.

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Structural, textural, surface chemistry and sensing properties of mesoporous Pr, Zn modified SnO₂-TiO₂ powder composites

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The Pr, Zn modified SnO₂-TiO₂ powder composites with mesoporous structure, was synthesized by a modified sol-gel method involving Tripropylamine (TPA) as chelating agent, TritonX100 as template and Polyvinylpyrrolidone as dispersant and stabilizer, respectively. The structural properties of the samples calcined at 600 °C and 800 °C were assessed by X-ray diffraction. N₂ adsorption/desorption isotherms were found to be characteristic for mesoporous materials, showing relatively low values for the specific surface area (15-32 m²g⁻¹) and nanometric sized pores. In case of the sample calcined at 800 °C, a bimodal pore size distribution can be observed, with maxima at 20 and 60 nm. SEM micrographs show a porous nanocrystalline morphology stable up to 800 °C. The surface chemistry was investigated by XPS. At 800 °C a diffusion process of Sn from surface to the subsurface/bulk region accompanied by a segregation of Ti and Zn to the surface is noticed, while Pr content is unchanged. The sensing properties of the prepared powders for CO detection have been tested in the range of 250-2000 ppm and working temperatures of 227-477 °C.

Structural and optical characterization of doped TiO₂ films

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The purpose of this work is to study multilayer TiO₂ films doped with Nb or V, obtained by successive deposition using the sol-gel-dipping method on the glass and Si substrates. The molar ratio TiO₂: Nb₂O₅ or V₂O₅ was 98:2 corresponding to an atomic ratio of 1.2 at.%. Thus it has been found that films doped with low amount of Nb/V are one of the efficient ways to obtain improved CO sensing performances. X-ray diffraction patterns show that the films are crystallized in the anatase phase. The optical properties have been systematically investigated by spectroscopic ellipsometry. The spectral dependency of the optical dielectric constant has been determined by modeling with the Oscillators. The surface roughness has been measured by atomic force microscopy and has been taken into account in the ellipsometric model. Since doped-TiO₂ films have a porosity greater than undoped TiO₂ films this explains their good behavior as CO sensor.

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Influence of the microwaves on the TiO₂ based sol-gel processes and on the properties of the resulted nanostructures

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The influence of the microwaves on the sol-gel process and on the properties of the resulted nanostructures (films or powders) are presented for the case of undoped and V doped TiO₂ systems. The reagents were tetraethyl orthotitanate, vanadyl acetylacetonate and ethanol was used as solvent. The starting solutions were homogenized either by stirring for 2 hours or were exposed to microwaves (MW) for 5 min at 300 W and a frequency of 2.45 GHz. Significant differences in the properties of the resulted films were noticed in the case of microwave assisted sol-gel method. The films presented a compact and continuous structure with very low roughness. The thickness of the films was higher showing close refractive indexes and increased transmission. In the case of the powders preparation, a significantly higher thermal stability of the gels obtained in the presence of the microwaves was observed. In the same time the V-doped TiO₂ powders prepared by microwave assisted sol-gel method presented an opposite sensibility for the water splitting and methanol oxidation.

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Erbium doped-SiO₂-TiO₂ or -SiO₂-TiO₂-Al₂O₃ nanopowders prepared by sol-gel method

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The Er³⁺ doped silica – titania or silica - titania - alumina nanopowders were prepared by sol-gel method that represents one of the most flexible and convenient way to prepare oxide films and nanopowders. The selected molar compositions were 90%SiO₂-10%TiO₂ or 85%SiO₂-10%TiO₂-5%Al₂O₃ and 0.5%Er₂O₃. Similar compositions were used for obtaining films for waveguides applications but the mechanism of the phase formation by thermal treatment of the corresponding gels was not previously approached. The gels obtained by the gelation of the solutions were analyzed by DTA/TGA in order to determine their thermal behavior and by IR spectroscopy to evaluate their structural evolution. The gels were thermally treated at temperatures higher than 500°C.

The thermally treated powders were characterized by Scanning Electron Microscopy (SEM), IR spectroscopy (FT-IR), X-ray diffraction (XRD) and photoluminescence (PL).

Synthesis, structural properties and photocatalytic behavior of ZnO powders prepared by sol-gel method

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ZnO powders have been prepared by sol-gel method starting from zinc acetate dihydrate as Zn source, triethanolamine as chelating agent and catalyst, and absolute ethanol as solvent. The molar ratio zinc acetate / triethanolamine was 5/1. After magnetic stirring for 2h at 50°C, the obtained solution left at room temperature. The characterization of the ZnO powders was made by TG/ATD analysis, X-ray diffraction and FT-IR spectroscopy. The ZnO - wurtzite phase was evidenced by XRD investigations. In addition, the Zn-O characteristic vibration band at 436 cm⁻¹ has been observed by FT-IR. For photocatalytic investigation the resulted powders were where thermally treated at 400 and 500°C for 1h. The photocatalytic tests have been performed in a quartz photo-reactor looking for Rhodamine B degradation under simulated solar irradiation, the transformation degree of the dye being 55% after 3h reaction.

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Ellipsometry study on TCO thin films used in optoelectronic applications

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In recent years we have studied different TCO materials (such as ITO, ZnO and Nb/V doped TiO₂) due to their unique properties of conductivity and transparency, in order to obtain thin films suitable for applications in optoelectronic devices and solar cells.

In this work Spectroscopic Ellipsometry (SE) is used as a powerful optical method for the characterization of these TCO films. Their optical properties were investigated in the spectral range of 190 - 1700 nm using a variable-angle spectroscopic ellipsometer from J.A. Woollam Co, Inc.

To simulate the experimental ellipsometric data, different models were used and a good agreement between measured and simulated data was achieved by taking into account the main characteristics of the films such as anisotropy, index grading, non uniformity etc. The thickness and optical constants of the samples have been determined and are consistent with the literature.

The surface roughness values obtained by SE are confirmed by Atomic Force Microscopy (AFM) investigations.

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**Influence of the substrates
on the sensing properties of the Zn-doped SnO₂ thin sol-gel films**

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Multilayered nanostructured thin films based on Zn-doped SnO₂ were prepared by dip-coating sol-gel method and deposited on glass, porous alumina, Si/SiO₂ and Si/SiO₂/Au wafers. The structure and morphologies of obtained films were investigated by scanning electron microscopy (SEM), X-ray diffraction (XRD), atomic force microscopy (AFM) and the gas sensing properties were evaluated. The gas sensing measurements performed for humidity and methane. The obtained results depend on the substrate used that influenced the structure and morphologies of the films.

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Rhodamine based fluorescent powder probes for Cu⁺² detection

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Rhodamine (Rh B) based fluorescent powder probes were obtained for the recognition of Cu⁺². The dye was immobilized in a silica matrix, generated by the co-condensation of tetraethylorthosilicate with its methyl and phenyl derivatives, using the sol-gel method. Compositional and structural characteristics of the Rh B-silica composites were determined and the influence of the organic substituents of the silica network on the properties of the Rh B-silica system was studied. Fluorescence tests were performed in the presence of Cu⁺². The fluorescence intensity of the composite probes strongly decreased in the presence of copper ion, more significantly in the case of Me and Ph-substituted matrices. A colorimetric response was also detected.

Effect of chitosan on the regeneration of tooth enamel using emdogain gel bioactive template

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Recent results show that amelogenin-chitosan hydrogel could acts as precursor for hydroxyapatite enamel crystallization in dental restoration applications. The paper presents the use of chitosan-emdogain-calcium chloride hydrogel as biomimetic precursor for in situ growth of remineralized enamel on an acid-etched dental enamel surface, by incubation in a phosphate solution containing fluoride, at 37 °C for 2-10 days. Emdogain gel is a commercial product used in tissue engineering, consisting in enamel matrix proteins premixed with propylene glycol alginate.

The size, orientation, structure and composition of remineralized crystals grown on the demineralized dental enamel surface were studied by scanning electron microscopy coupled with energy dispersive x-ray spectrometry (SEM-EDS), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy and X-ray diffraction (XRD). SEM-EDX results showed that the remineralized enamel crystals grown on the demineralized enamel surface are apatite hexagonal structures. Raman, XRD and FTIR data confirmed the fluorinated hydroxyapatite phase, which degree of crystallization increases with increasing duration of synthesis. The effect of chitosan on the above mentioned characteristics of the obtained remineralized layers was investigated.

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titanium	S8-Poster (<i>Predoană et al.</i>)	WQI	S6-Poster (<i>Timofti et al.</i>)
titanium	S4-Poster (<i>Marcu et al.</i>)	X-ray analysis	S1-Poster (<i>Baratoiu-Carpen et al.</i>)
titanium	S4-Poster (<i>Vasilescu et al.</i>)	X-ray photoelectron spectroscopy	S5-Poster (<i>Tudose et al.</i>)
titanium aluminide	S5-Poster (<i>Banu et al.</i>)	XPS	S4-Poster (<i>Preda et al.</i>)
titanium dioxide	S2-Poster (<i>Neacsu et al.</i>)	XPS	S6-Poster (<i>Enache et al.</i>)
titanium hydride	S2-Poster (<i>Sofronia et al.</i>)	XRD	S2-Poster (<i>Rusti et al.</i>)
transmission characteristics	S8-Poster (<i>Barton et al.</i>)	yttrium doped supports	S7-Poster (<i>Ilieva et al.</i>)
transmission electron		zeta potential	S2-Poster (<i>Neacşu et al.</i>)
		Zinc oxide	S6-Poster (<i>Cucoş et al.</i>)
		zinc oxide	S6-Poster (<i>Vişinescu et al.</i>)
		Zinc-Titanium-Iron mixed oxides	S7-Poster (<i>Hornoiu et al.</i>)
		Zn(II)	S5-Keynote (<i>Paraschiv et al.</i>)
		Zn-doped SnO₂	S8-Poster (<i>Tenea et al.</i>)
		ZnO	S5-Poster (<i>Hristea et al.</i>)
		ZnO	S5-Poster (<i>Paraschiv et al.</i>)
		ZnO	S8-Poster (<i>Stoica et al.</i>)
		ZnO nanoparticle	S7-Poster (<i>Chelu et al.</i>)

KEYWORD INDEX

ZnO based films

S5-Poster (*Mihaiu et al.*)

ZnSe

S5-Poster (*Tigau et al.*)

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Vasile Voiculescu (1884-1964)
Pescarul Amin / The Fisher Amin

*Si alaiul fabulos al pestilor se desfasura triumfal, la mijloc cu
morunul fantastic inconjurat de cetele genunilor, ducând la piept
pe stranepotul sau, pescarul Amin, într-o uriasa apoteoza catre
nepieritoarea legenda cosmica de unde a purces dintotdeauna, omul.*

*And the fabulous fish cortege unfolded in triumph, with the fantastic
sturgeon in the middle surrounded by the abyssal cohorts, carrying
his great-grandson, the fisher Amin, in a vast apotheosis towards
the unfading cosmic legend wherefrom man ever emerged.*

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