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Abstracts

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CP1. The beauty of coordination polymers

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Crystal engineering of coordination polymers represents one of the most fascinating fields in modern chemistry. It encompasses both inorganic and organic synthesis. The metal ions, through their stereochemical and electronic predilections, play a key role in controlling the assembly of the molecular components into well-defined architectures.[1]The ultimate goal of crystal engineering is to design solids with technologically useful functionalities (molecular magnetic materials, conducting solids, zeolite-like materials, catalysts, luminescent materials, etc.). Originating from Robson's seminal papers published in 1990,[2] the node-and-spacer approach became a largely employed strategy for the construction of a rich variety of coordination polymers. It relies upon the strong directionality of the coordination bonds established between the metal ions (nodes, connectors) and the *exo*-dentate ligands (spacers, linkers).

We enlarged the classical node-and-spacer approach employing homo-and heterometallic complexes as nodes.[1,3] Several families of such compounds synthesized recently in our Laboratory will be presented in this lecture.[4]

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CP3. Biosensors for dopamine determination in foods of plant origin

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Research and development of novel method for analysis have as objective to combine sensitivity, precision, accuracy and selectivity with rapidity, simplicity and low cost.[1] For this reason, the importance in developing biosensors has increased in the last years.[2]

In this study, tyrosinase has been immobilized on a mesoporous carbon modified screen-printed carbon electrode for the estimation of dopamine. Tyrosinase maintains its biocatalytic activity well on carbonaceous thin film. The biosensor was characterized by cyclic voltammetry and amperometry. The analytical and performance characteristics of biosensor, including sensitivity, linear range, detection limit and repeatability have been achieved. The principle of dopamine detection was based on the reduction of biocatalytically generated quinone derivatives at -0.15 V versus Ag, with good sensitivity and selectivity. The kinetics of the enzymatic reaction fitted into a Michaelis-Menten type kinetic. Different parameters influencing biosensor performance have been optimized including applied potential, pH and temperature. The response of biosensor had a linear relationship with the concentration of dopamine in a wide range of (0.05 μM-120 μM), with a low limit of detection (0.02 μM). Selectivity of biosensor towards interfering compounds has been also studied. Determination of dopamine amounts in foods of plant origin has been shown good recovery in the range of 99-101%.

Acknowledgments:
This work was supported by a grant of the Romanian National Authority for Scientific Research, CNCS - UEFISCDI, project number PN-II-ID-PCE-2011-3-0255.

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CP4. New materials with application in Oenology

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The realities of modern winemaking require the scientific development of some technological decisions based on the new concepts to control the production of different wine types.

The alternative approaches of wine treating and conditioning for removing metal ions, phenolic compounds, biogenic amines or volatiles are scientific attempts to improve quality of wines during the cycle of wine production.

Current evaluations of the adsorbents properties used as oenological materials show advantages and disadvantages such as selectivity of action, environmental and economic elements.

For this reason, among the new research directions are the actions of new materials on the physico-chemical composition and organoleptic properties of wines which has led to valuable results published in national and international journals.

CP5. Organometallic compounds as building blocks for supramolecular architectures

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Organometallic compounds in which a number of functionalized organic groups are attached to a central metal atom can be used as robust, air stable neutral or anionic tectons. Depending on the nature of the metal, the organic groups bearing recognition sites and anionic groups able to behave as bridges between different metal atoms (e.g. thiocyanate, azide), ditopic, tritopic or tetratopic tectons can be obtained. Symmetric/asymmetric ligands with appropriate distance between the recognition sites can be obtained and used as required for the network designed to be obtained. In addition, organometallic species exhibiting different types of chirality can be obtained; in some cases the presence of a lone pair of electrons might bring useful properties. Examples of such organometallic tectons based on a main group metal (Sn,[1,2] Sb,[3,4] Bi[4]) or mercury[5] will be presented and discussed as well as some transition metal complexes and supramolecular solid-state architectures of different dimensionalities (linear coordination polymers or 3D networks) built on the base of various supramolecular interactions.

Acknowledgements:
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CO1. Clinical diagnostics of lysosomal storage diseases on dry blood spots: MRM-MS and fluorimetric determinations

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The loss of enzyme activity is a characteristic feature of lysosomal storage diseases (LSDs), a group of ca. 70 metabolism disorders such as mucopolysaccharidoses, sphingomyelinoses, and neuronal ceroid lipofuscinoses. Defect of enzymes cause substrate accumulation in lysosomes, leading to severe disease symptoms and finally death. For several LSDs treatment has become available by enzyme replacement therapy (ERT), however, successful ERT is critical to start early which renders clinical diagnostics of key importance. Accumulation of glycosaminoglycans within lysosomes can produce progressive cellular damage leading to skeletal malformations, pulmonary deficits, short stature, retarded growth, hepatic and cardiac abnormalities and sometimes neurological abnormalities[1]. Neuronal ceroid lipofuscinoses (NCLs) are a group of the most common neurodegenerative disease in childhood, characterized by dementia, epilepsy, and progressive physical decline and early death of patients. From mucopolysaccharidoses diseases MPS II, known as Hunter disease and MPS VI, known as Maroteaux-Lamy syndrome are the most common MPSs[2]. We optimized enzyme reaction condition and procedure for the assay, including concentration of substrates and internal standard, composition of extract buffer and mass spectrometer parameters. Clinical diagnostics assays were developed by MS-MRM determinations with an Esquire 3000 ion trap mass spectrometer (Brucker, Germany).

Acknowledgment:
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CO3. Investigations on the isoprene ozonolysis: Product yields formation over temperature range 273-343 K

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The atmosphere is a complex mixture of gases and particles with high impact on the climate and human lives. The most abundant biogenic volatile organic compound (BVOC) is isoprene with 500 Tg annual emissions.[1] The isoprene oxidation process in the atmosphere is very complex and despite years of research studies, the degradation mechanism is still poorly understood, especially in remote area described as low NOx environments. The main primary carbonyl products formed from the ozonolysis of isoprene include methacrolein (MACR), methyl vinyl ketone (MVK) and formaldehyde.[2] As ozonolysis of alkenes in gas phase is an important source of HO_x via the Criegee mechanism, precise experimental determination of OH and HO_2 from isoprene ozonolysis is of the utmost importance.

This study will present for the first time the temperature dependent experimentally determined product yields from the ozonolysis of isoprene (using CO and cyclohexane to scavenge >97% OH radicals). The experimental data are compared with the yields predicted from a model based on the Master Chemical Mechanism (MCM). The study follows the formation yields of MACR, MVK, formaldehyde, OH and HO_2 radicals over the range 273–343 K in the HIRAC (Highly Instrumented Reactor for Atmospheric Chemistry) chamber.[3] The HO_2 yield determined using FAGE (Fluorescence Assay by Gas Expansion)[4] is measured at low RO_2 interference contribution (< 5%).

OH formation yields were determined using different methods: *i*) pseudo first order kinetic experiments in the presence and absence of an OH scavenger; *ii*) a tracer method and *iii*) direct observations using FAGE instrument and fitting the OH temporal profile.

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CO7. Ethics in science, chemistry and academia.

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The contribution takes in consideration several professional and moral standards, applied generally in science and particularly in chemistry, with relevance for the relation between science and society. Aspects related to synergism and antagonism involving the categories *ethics, education, law, politics* and *religion* are discussed. The relation between scholars and master, the research national and international system, as well as the education system in high schools and universities are taken in account as key points in the formation of young researchers and scientists. The importance and the relevance of the contribution of mass media in science are also mentioned.

CO8. Template assembles of single molecule magnets based on manganese coordination compounds

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The coordination chemistry of the transition metal compounds containing thiosemicarbazide derivatives are investigated due to their attractive chemical, physical and biological properties. Using various thiosemicarbazide derivatives and different metal ions in different oxidation states, allows the preparation of a large number of coordination compounds with original structures and properties.

Cyanide is an efficient and versatile mediator for magnetic coupling. The cyanide- bridged bimetallic assemblies have been widely studied because of their rich magnetic behaviour.[1] Miyasaka et al. have prepared a series of cyanide-bridged products derived from the reaction of manganese (III) Schiff Base coordination compound and hexacyanometalate anions.[2]

Here we describe a new family of isostructural linear trinuclear compounds $[NEt_4\{[Mn(L)]_2[M(CN)_6]\}$ (M = Fe, Ru, Os) (Figure 1.a) obtained from anisotropic building-block based on manganese(III) compound and 3d, 4d and 5d hexacyanometalate unit. AC-magnetic measurements were show that compounds have slow relaxation of magnetization at low temperatures (Figure 1.b).

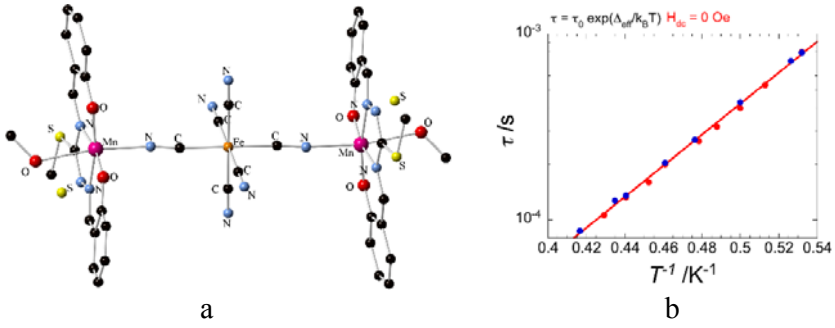

Figure 1: (a) Crystal structure of the Mn-Fe-Mn. The NEt_4^+ counter ion and H atoms have been omitted for clarity. (b) Arrhenius plot of the ac magnetic behaviour of the trinuclear compound

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CO10. Oxytetracycline delivery systems based on mesoporous titania

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Titania, a well-known biocompatible material, could be employed in drug delivery systems (DDS) and most studies referred to TiO_2 nanotubes as inorganic vehicle for biologically active molecules.[1,2]

The aim of our work was to obtain mesoporous titania with different structural and textural properties by solvothermal method and to employ these inorganic materials as vehicles for oxytetracycline, a broad-spectrum antibiotic. The drug loaded samples were prepared by incipient wetness impregnation method that is an efficient, simple and reliable technique to obtain DDS. In the wide-angle XRD patterns of all drug-loaded materials, only the Bragg reflections of anatase phase belonging to the support were noticed proving that the drug was adsorbed into the carrier mesopores in amorphous state. The BET specific surface area, total pore volume and average pore diameter values for the mesoporous titania samples were in the range of 109-274 m^2/g, 0.30-0.44 cm^3/g and 3.72-10.16 nm, while for the corresponding oxytetracycline-loaded materials, lower values were measured ranging in 17-65 m^2/g, 0.04-0.14 cm^3/g and 3.71-9.03 nm.

The oxytetracycline delivery profiles, performed in phosphate buffer solution (pH=5.7) at 37°C, exhibited a burst effect, about 40% of adsorbed antibiotic was released in the first 10 minutes of the experiment, followed by a gradually drug delivery (up to 6 h) depending on the carrier textural properties. Slower delivery kinetics was observed for the samples containing calcined titania than for the materials comprising TiO_2 purified by extraction, demonstrating the existence of strong interactions between titanium ions and drug molecules.

Acknowledgment:
The Romanian project PCCA no. 131/2012 is gratefully acknowledged.

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CO12. Intermolecular interactions and spin crossover materials

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Among the coordination compounds, the spin crossover compounds are the most representative examples of the molecular bistability. In the case of Fe(II), is possible to switch the system between the paramagnetic (high spin S = 2) to diamagnetic (low spin S = 0) state and vice versa. This phenomena implies significant magnetic, structural, electrical, chromatic and optical modifications. This open up a plethora of potential applications in the fields of display, memory[1], nanoscience[2] as well as in the other areas… Beside the fact that this phenomenon is known since 1931[3] and hundreds of compounds were studied, just handful show bistability properties around room temperatures required for device applications.[4] The transition temperature and coopertivity of a SCO system are depending of intermolecular interactions in the crystal lattice and also by molecules themselves.[5]

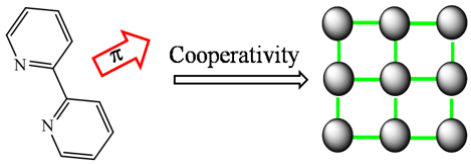

Figure 1. Schematic representation of organic ligands involved in this work, (bpy = 2,2' – bipyridine) and increasing of cooperativity through π-π interactions.

Here we study the influence of π-π interactions on the spin transition properties in few families of Fe(II) compounds. The π-π interactions are assured by including organic ligands with different number of aromatic rings and different solvents. Also, we show the influence of solvent insertion in the crystal lattice on the intermolecular interactions and transition properties.[6] We observe that the number of aromatic rings involved and different solvents influence differently the cooperativity and transition properties in different classes of studied materials.

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SC7. Mesostructured silica and aluminosilicates as carriers for irinotecan delivery systems

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Mesoporous silica and aluminosilicate nanoparticles meet the requirements of being employed as drug carriers due to their good storage capacity arising from their appropriate porous nature (ordered pore array with narrow size distribution, high surface area and pore volume) and to their non-toxicity and biocompatibility.[1,2] The drug - matrix interactions can be tailored by tuning the structural and textural features of these materials, leading to an appropriate adsorption and a predictable release profile.[3]

Four SBA-15 and AlMCM-41-type mesostructured materials were employed for the design of new delivery systems for irinotecan, an anticancer agent. The influence of the structural and textural properties, as well as the aluminum incorporation into silica matrix were investigated with respect to irinotecan adsorption and its release in simulated body fluids: phosphate buffer solution, pH=5.7 and Ringer solution. The main mechanism involved in the desorption process was proved to be a Fickian diffusion and the *in vitro* release profiles were found to be clearly dependent on the carriers characteristics. The cellular proliferation tests, performed on NIH3T3 murine cell line, indicated an enhanced toxicity of irinotecan-loaded mesostructured inorganic carriers as compared with the drug alone, while the supports did not modify the cell proliferation rates. Confocal microscopy images suggest a vesicular-mediated incorporation of the carriers explaining the cytotoxicity augmentation when the therapeutic agent is loaded on mesostructured inorganic supports.

Acknowledgment:
The Romanian project PCCA no. 131/2012 is gratefully acknowledged.

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P1. Differential pulse anodic stripping voltammetry in mercury determination

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In the present work voltammetric investigations have been performed on $HgCl_2$ aqueous solutions prepared from a Cz 9024 reagent. Carbon paste electrode (CPE), eriochrome black T modified carbon paste electrode (MCPE/EBT) and KCl 1M as background electrolyte were involved within the experimental procedures. Cyclic voltammetry (CV) has been performed in order to compare the behavior of the two electrodes in both $K_3[Fe(CN)_6]$ and mercury calibration aqueous solution. Differential pulse anodic stripping voltammetry (DPASV) helped in determining the most suitable parameters for mercury determination. All experiments were performed at 25 ± 1 °C, using an electrochemical cell with three-electrodes connected to an Autolab PG STAT 302N (Metrohm-Autolab) potentiostat that is equipped with Nova 1.11 software. The measured potential values were generated by using as reference the silver chloride electrode (AgClE) and as auxiliary a platinum wire electrode. A series of time depending equations for the preconcentration and concentration steps were established, with the observation that an increased sensitivity can be obtained while increasing the preconcentration time. DPASV were drawn using the CPE in 11.16% coriander, as mercury complex, the voltamograms signals indicating mercury oxidation, with signal intensity increasing in time.

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P2. Sm(III) polyoxometalate: synthesis, structure and properties

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A new polyoxometalate Sm(III)-$W_5O_{18}^{6-}$ has been synthesized and characterized by DRX, IR, DTG techniques. The catalytic activity of the obtained compound is studied for the decomposition of hydrogen peroxide, and the effect of the reaction time, the catalyst amount, solvent polarity and volume of hydrogen peroxide are investigated by volumetric method.

The structure was solved by the direct method and refined by the full-matrix least squares method on F^2 using SHELXTL 97 crystallographic software package.

The compound was crystallized in the triclinic system, space group P-1 with a = 12.8119(5) Å, b = 113.1373(6) Å, c= 20.5709(9) Å, α = 82.737(4) °, β = 74.808(4) °, γ = 89.036(3) °, V = 3314.07 $Å^3$, Z = 2.

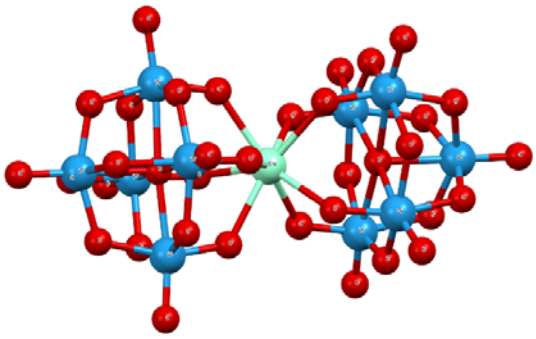

Figure 1. Crystal structure of $[Sm(W_5O_{18})_2]^{9-}$.

The obtained results recommend the use of this compound as catalyst in the decomposition reaction of the hydrogen peroxide.

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P4. Comparative Photodegradation Study of Erythrosin B Using Two Reactors Type

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The photodegradation of Erythrosin B was studied in two different reactor types: slurry and suspended reactor (SSR) (Caliman et al.) and fixed bed reactor (FBR) (Pereira et al.). The main differences between the operating of the two reactors consist in the catalyst amount and the arrangement and irradiation supply details, provided by different UV lamps. For the studied conducted in the reactors the catalysts used were: Degusa TiO_2 Aeroxide P25 with 80 / 20 weight ratio of anatase/rutile for SSR, and the rutile form type Tiona PC500 TiO_2 for FBR, respectively.

In the SSR, a concentration of $5 \cdot 10^3$ mg L^{-1} of Degussa TiO_2 Aeroxide P25 catalyst was used and the particles were kept in suspension. In the FBR, the catalysts was arranged by compression in a fixed non-woven fabric made of cellulose fibers, reaching concentrations values of respectively 16.2 mg L^{-1} Tiona PC500 TiO_2, 1.8 mg L^{-1} Snowtex 50 SiO_2 and 0.18 mg L^{-1} UOP 2000 zeolite. The values of reaction rates were 0.2716 mmol L^{-1} h^{-1} in FBR and 0.0887 mmol L^{-1} h^{-1} in SSR, respectively. In the case of TiO_2 arranged in FBR, Erythrosine B photodegradation was faster in the first hour of the process. The resulted removal efficiencies were around 90% in both reactors. The pH in the two reactors follows different behaviors: in the fixed bed reactor it increases from 6 to 7 during the first 9h of reaction, in contrast to the slurry reactor where pH values decrease from 6 to 4. The feasibility of TiO_2 recycling in the SSR was carried out after adsorption and degradation test. The activity of the catalyst decreased starting with the second cycle with around 15%; the next cycle showed a degradation rate with around 38% lower that the first cycle. The fourth cycle indicated that the TiO_2 activity is halved.

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P5. Magnetic mesoporous inorganic composites with biomedical applications

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Ferrite-based composite materials have many applications in biomedicine, catalysis, magnetic separations, etc. Generally, pristine magnetite nanoparticles (NP) have the tendency to aggregate in large agglomerates due to anisotropic dipolar attraction and in order to avoid this drawback they should be embedded in a biocompatible material as polymers[1] or mesoporous silica.[2] Unlike Fe_3O_4, cobalt ferrite has high oxidation stability and due to its similar magnetic properties and low toxicity could replace successfully iron oxide NP.[3]

Composite materials consisting in magnetite or cobalt ferrite nanoparticles with the sizes in the range of 7-12 nm encapsulated in mesoporous MCM-41-type matrix with an ordered hexagonal pore array were obtained by two procedures: one pot approach and two steps synthesis. The first method led to a higher content of ferrite NP, but a less ordered pore framework of silica matrix than the second approach.

All the composites exhibited superparamagnetic behavior, enough high saturation magnetization (1.26-3.77 emu/g) and high porosity (S_{BET} in the range of 600 -784 m^2/g), features that are necessary for biomedical applications.

Acknowledgment:
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P6. Mesoporous silica-ceria composites as carriers for drug delivery systems

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Ordered mesoporous silica could be combined in a composite or hybrid material with inorganic or organic compounds, in order to design advanced functional materials that gather the advantages of both components of the composite. Mesostructured silica was reported as a carrier for several active pharmaceutical ingredients due to its outstanding properties: ordered pore array with tunable pore dimension, high surface area and total pore volume, as well as biocompatibility.[1] Nanoceria exhibits radical scavenger properties as a consequence of the interconversion of $Ce^{4+} \leftrightarrow Ce^{3+}$ on nanoparticles surface and could be applied as therapeutic agent for hart, retina or neurological diseases.[2]

Herein, we report the synthesis and characterization of mesoporous silica-ceria composites with an ordered hexagonal pore array characteristic to the MCM-41 materials, which were applied as carries, besides MCM-41 silica matrix, for oxytetracycline that is a broad spectrum antibiotic. The inorganic mesoporous matrices and antibiotic-loaded samples were characterized by various techniques: small- and wide-angle XRD, FTIR spectroscopy, N_2 sorption analyses, as well as SEM and TEM. The drug delivery profiles were determined in phosphate buffer solution, pH = 5.7. All drug release profiles exhibited a pronounced burst effect, but slower kinetics was noticed for oxytetracycline delivered from mesoporous silica-ceria composites.

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P7. Chemistry expertise of polymeric supports from the counterfeit documents

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Chemical composition of the counterfeited document material can be evaluated through chemical expertise of the document supports. The role and preservation of these documents have a close connection with the evolution of society. Physico-chemical expertise of the documents established chemical nature of the materials, their conservation status, archaeometry, artofactometry and chemometrics characteristics. Also physic-chemical expertise by characterization scriptural and materials supports is an important instrument in authentication of the document discrimination from the forged that, an important means of proofing of forgery and counterfeiting document, and checking of the default identity cards as well. Therefore this study presents the evaluation of the physico-chemical properties of the polymer support of different identity cards suspected to be forged or counterfeit, the comparison being made with a standard sample of a genuine document.

For the achievement objectives were selected a few forget identity cards of which small samples were taken and a standard sample of the model document comparator (specimen). Samples have been analysed involving the microscopic techniques spectrophotometric measurements such as micro FTIR (HYPERION FT-IR microscope, Bruker Optics Courtey) and scanning electron microscopic coupled with Energy Dispersive Analysis X-ray Spectroscopy (SEM-EDX) to determine the nature of the polymers of genuine supports and from the counterfeit.

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P8. Synthesis of polymetallic oxides with high organized structure

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Polymetallic oxides with spinel type structure are compounds with the general formula AB_2O_4 where A is a divalent metal (i.e. Ni^{2+}, Mn^{2+}, Zn^{2+}, Co^{2+}, Cu^{2+}) and B is the trivalent metal (i.e. Fe^{3+}, Mn^{3+}). In the spinel-type structure, the metal cations can occupy tetrahedral (A) and/or octahedral sites [B] inside a compact pseudo-cubic lattice packing. These compounds are characterized by chemical and thermal stability that make possible to be used in various applications, such as catalysts and gas sensors, data storage devices and/or recovery of information, microwave devices, in biomedical applications as contrast agents in diagnosis and magnetic-guided devices for targeted and pulsed release of active principles, as pigments, anodes for Li-ion batteries etc.[1,2,3]

In this paper are presented the comparative results obtained for $NiFe_2O_4$ samples synthesized by sol-gel autocombustion method, using glycine as chelating/fuel agent and polyacrylamide-based hydrogel as template agent. In specialized literature it is noted that polyacrylamide-based hydrogels can be used for obtaining coated Fe_3O_4 nanoparticles. Also, hydrogels can be used as possible template agents for obtaining nanometer-size oxidic compounds displaying highly organized structure.

The synthesized samples were structurally characterized by IR spectroscopy, XRD and SEM. IR spectroscopy was applied for tracking the disappearance of the organic and nitrogen phases, and also for monitoring spinel structure formation. XRD technique was used to confirmation of the spinel-type structure and single phase formation of the as- obtained samples. SEM was used for confirmation of the high organized structure.

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P9. Rhodamine 6G dye photodegradation study on TiO_2 –based photocatalysts

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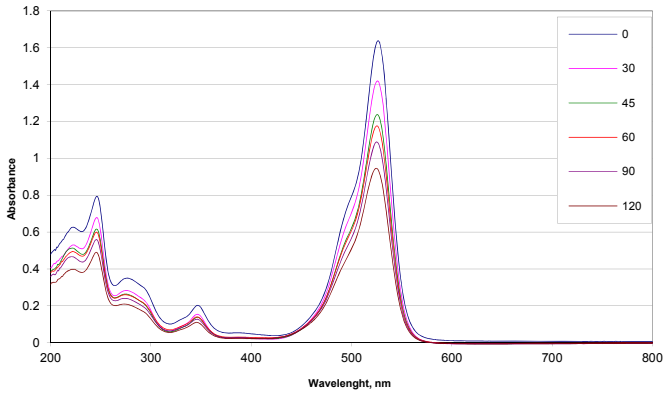
The photodegradation of Rhodamine 6G (R6G) dye study was made on 3 types of solids: mesoporous TiO_2, CeO_2 and WO_3 - doped TiO_2 by the Incipient Wet Impregnation (IWI) technique. The mesoporous titania was prepared by the evaporation induced self assembly (EISA), using titanium isopropoxide, hexadecyl-trimethyl-ammonium bromide (CTAB), HCl, ethanol and water. The removal of the template was performed by calcination at 450˚C (1^o/min) during 2 h. The solids were characterized by the BET adsorption of nitrogen, which confirmed the porous structure and high values of specific surface areas. The photocatalytic tests were performed in a stirred photoreactor, under UV irradiation, using a lamp immersed in the middle of a quartz tube placed in the reactor.

The behaviour of the solids in the photodegradation of R6G strongly depends on the pH value of the reaction medium and also on the photocatalyst dose and initial dye concentration. Remarkable results were noticed on the mesoporous TiO_2, when working at pH value of 6, using a solution of 30 ppm of dye, at a photocatalyst dose of 0.3 g/L; a conversion degree of 94 % was found after 2 hours of irradiation with UV.



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P10. Morphological and microchemical surface analyses of modern coins minted in the 20th century

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Scanning electron microscopy (SEM) coupled with energy dispersive X-ray analyser (EDAX) are non-destructive analytical techniques suitable for the investigation of specific features in various materials. These techniques bring significant contribution also in numismatic area where sample integrity is of great importance [1-3]. In the present work fifteen coins of various origins (Romania, Germany, Bulgaria, Poland, Russia and United States of America) minted in the 20th century were subjected to microchemical surface analysis. Analyses has been undertaken after gentle cleaning of the samples with methanol:ethanol mixture (1:1 ratio) to preserve samples integrity. SEM analyses revealed the existence of important morphological details in the investigated coins (*i.e.* surface defects, corroded areas, deeply penetrated solid particles). Investigations performed on EDAX clearly showed that major elements abundance (Ag, Cu, Ni, Zn) is highly correlated with coins origin area and their minting period. Minor identified elements such as C, O, Fe, suggests either the influence of contamination or the existence of some oxides or hydroxyl groups on coins surface. Use on purpose of some elements to improve alloys properties might be another cause. The results obtained within the present work highlighted that tracer elements can be specifically assigned with the major aim to help in numismatic objects historically dating.

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P11. Dinitrophenolic pollutants in the environment: toxicity and decontamination

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Numerous hazardous chemicals from various industrial sources or agriculture enter into environment daily.[1] Many compounds are frequently used as drugs, pesticides or dyes. For example, many of these compounds, including 2,4-dinitrophenol (2,4-DNP) and derivatives, 4,6-dinitrocresol (DNOC) or 2-sec-butyl-4,6-dinitrophenol (Dinoseb) are widely used pesticides that may persist in the contaminated soils. Consequently, several decontamination methods envisaged removal of refractory pollutants from contaminated area, to circumvent their transfer through food chain.[2]

The results suggest that yeast (*Saccharomyces cerevisiae)* could be used as a genuine biodegradation agent in the contaminated environments with dinitrophenol pesticides and related compounds.[3] The yeast-associated microbiological degradation can be applied in the case of uncoupling dinitrophenols, whereas phytoremediation may be recommended to other pollutants.

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P12. Adsorption of some organic compounds of biological interest from wine on mesoporous solids

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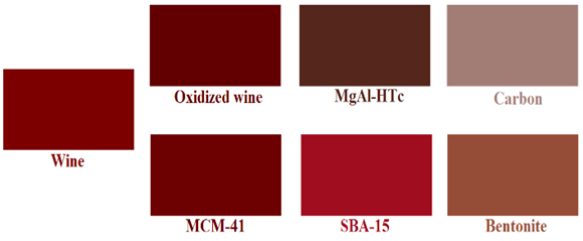
In the present work we aimed to compare the adsorptive properties of several solid mesoporous materials in the uptake of some active biologic compounds from red wine (Cabernet Sauvignon). The tested materials were: mesoporous silicas SBA-15 and MCM-41, a synthetic anionic clay (MgAl-HTc) and the usual adsorbents used in the wine industry, sodium bentonite and active carbon.

The adsorption consisted in the stirring for one hour of a wine sample with the calculated amount of solid at room temperature, followed by letting the suspension in the fridge for about 20 h in static conditions, after that for 15 minutes was stirring.

After that the wine samples were analyzed using the UV-Vis, spectroscopy and the HPLC. The color of the wine samples after being contacted with the solids showed important changes, indicating the adsorption on the solid of the most of the colored compounds (see figure.). The colors from this figure were obtained by converting in RBG the individual UV-VIS spectra of the wine samples after being in contact with the solids. The solids were analyzed by FT-IR and DR-UV-Vis spectroscopy.



Important individual features were noticed for the behavior of the solids in the adsorption selectivity of the various compounds from wine.

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P14. Structural evaluation of biocomposite materials based on PVA and CNC

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This study was undertaken to evaluate the effect of different concentrations of cellulose nano-crystals (added as nano-reinforcement) and glycerol (plasticizer) on structural properties of PVA films, and to establish an optimum formulation to provide the best possible combinations of properties related to performance of the materials as food packaging.

Cellulose nano-crystals (CNC) were prepared by acid hydrolysis technique from the cotton wool. For the composite preparations three different concentrations of the CNC in the polymer matrix were used.

PVA/CNC composite films were prepared by solvent casting method. Their morphology was evaluated by scanning electron microscopy, whilethe structural properties were evaluated by UV-Vis and FTIR spectroscopy, and XRD.The obtained films are transparent – this fact being confirmed both by visual observation and by UV-Vis spectroscopy.The qualitative and quantitative differences which appear in the samples were evidenced by FT-IR spectroscopy. This technique indicates interactions through thehydrogen bondsbetween the OH groups of PVA and CNC. The IR spectra from the fingerprint region show characteristic bands for both components. Significant differences appear in the 1200-900 cm^{-1} spectral region.When the CNC content increase, an increase of the intensity of the band assigned to stretching vibrations of the C-O groups and C-O and C-C groups from glycoside ring and a decrease of the bands assigned to C–C and C-O groups from PVA take place.

Following the deconvolution process of the X-ray diffraction patterns, it was found that the degree of crystallinity tend to increase with the increasing of the content of CNC in the films.

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P16. Phytochemical variability of *Thymus pulegioides* L. wild populations from Eastern Carpathians

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Lemon thyme is an aromatic plant used both for medicinal purposes and as a spice almost all over the world. In the Romanian flora there grow 17 *Thymus* species, out of which 16 are spontaneous, and one (*Thymus vulgaris* L.) is cultivated.[1] In the essential oils belonging to the species of the *Thymus* genus, we noticed a great chemical variability.[2,3] 8 chemotypes are characteristic for the *Thymus pulegioides* L. essential oil[2]. In this study samples from 12 wild populations of *Thymus pulegioides* located along Bistrita River (Eastern Carpathian Mountains) were collected. A phytochemical analysis for various polyphenolics by chromatographic and spectrophotometric methods was performed. Also, a comparative GC-MS analysis of essential oils from one of the samples (Madei) with their mixture (collective drug). Chemical composition of the essential oils was established by gas chromatography coupled with mass spectrometry (GC/MS). The phenolic acid and flavonoid content of the *Thymus pulegioides* samples was estimated by means of a reverse phase HPLC-UV method.

In conclusion, the interpopulational variability is displayed at the level of essential oil build-up in *Thymi herba*; a major quantity of carvacrol was marked out in one of the wild populations (Madei) as compared to the collective drug of all the samples combined. Supplementary the analysed wild populations were characterized by a relatively low amount of thymol, thus the plant material could be used in formulae for food supplements.

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P17. (Bio)remediation of Heavy Metal Contaminated Effluents in Mechanical and Pneumatic Mixed Systems

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Water pollution with heavy metals became one of the most important and current problem for the environment, as a result of specific industrial activities, which use metals in various processes. These chemical species are considered inorganic persistent pollutants, with high bioavailability and capacity to be transported and bioaccumulated in the food chain, thus generating serious pollution problems for human health and ecosystems. Consequently, large efforts are invested to remove heavy metals form contaminated industrial effluents. Besides the conventional physico-chemical methods, which often proved to be unsustainable, biological methods (biosorption and bioaccumulation) are more and more considered feasible, environmentally friendly and often low-cost options. Different types of biomass (such as microorganisms, algae, agricultural plants and wastes) are used as low cost biosorbents and bioaccumulators for the bioremoval of heavy metals from contaminated effluents. Our studies address the application of biosorption and bioaccumulation of heavy metals by indigenous microorganism (bacteria and fungi) in different types of bioreactors. In this context, the purpose of this paper is to establish the steps and parameters (pH, biosorbent dose, contact time, pollutants concentration, temperature, liquid flow rate etc.) which influence biosorption and bioaccumulation processes applied in bioreactors, in batch and continuous mode. Although many types of contacting systems can be used for bioremediation, we focused on the analysis and comparison of heavy metals bioremoval performance in stirred tanks and airlift bioreactors.

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P18. Analysis of the Degradation and Potential Human Health Risks of Twelve Pesticides Applied in Double Dose in Tomatoes

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The objectives of our study were focused on a detailed assessment of the behavior of 12 pesticides (7 fungicides and 5 insecticides) applied on field-grown tomatoes. We have applied three treatments in double dose considering the phenological growth phases of tomatoes. The experiments were conducted within an experimental lot in the Mures Fitosanitary Unit (Romania). Tomatoes plants were transplanted in an open field on two rows to 0.6 m wide and 0.3 m distance between plants on the same row, at a density of 45-50 thousand plants/ha. Buffer areas have been ensured between the tomatoes plants subjected to the experiment. The pesticide residues in tomatoes were analyzed by an Agilent 7890 gas chromatograph coupled with a mass spectrometer with time of flight, CG*GC-TOF-MS Pegasus 4.21 (LECO, SUA). Degradation of pesticides residues was strongly influenced by temperature, humidity and precipitations which were monitored with a meteorological station Adcom Telemetry addAvantage type. The degradation results allowed us to estimate potential human health risks, for both adults and children, associated with the pesticide residues in vegetables at harvest. Human health risk analyses were based on the latest fruit consumption data released in 2015 by Freshfel Consumption Monitor of 188.60 g/capita/day, on average in 2013, for the EU-28. The lifetime exposure dose to pesticides (mg/kg/day) was calculated by multiplying the pesticide concentration in tomatoes at harvest and at two months after harvest in samples (mg/kg) with the food consumption rate (kg/person/day), and dividing the product by the consumer body weight (kg). The results of health risk analysis revealed that only the pesticide chlorothalonil can prezent a risk to human health, when applied in double dose.

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P19. Dynamic behaviour of organic pollutants in the soil matrix - the influence of main parameters

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The evaluation of the sorption/desorption processes of organic pollutants in different soil horizons is very important for understanding the fate, mobility and behaviour of these chemical species in soil, and provide useful data for assessing the potential environmental hazard associated with them. The purpose of this study was to investigate the processes of sorption and desorption of azo dyes in natural soils.

The experiments were conducted in dynamic mode. Column experiments were performed in order to reproduce field conditions, with the goal to obtain information which is not available from batch studies; so we investigated the influence of parameters, such as soil column height (Z), flow rate (Q) and initial concentration of the chemical in aqueous solution (C) on Congo red (CR) behaviour in soil. Several models such as Thomas, Adams–Bohart, Wolborska and Yoon–Nelson were applied to describe and predict the transport phenomena associated with the presence of Congo red in a soil collected from Iasi area (Romania). It was found that the dye is sorbed on the soil, while the sorption onto the investigated soil does not describe a typical S-shaped curve and the values of breakthrough time are very low. It was observed that, at low CR concentration, there is a relative slower transport determined by a declining in diffusion coefficient and mass transfer coefficient values. The saturation time is achieved earlier and the breakthrough time appears quicker when the initial CR concentration increases. These results demonstrated that any change in concentration gradients can affect the rate of saturation of the soil layers and the exhaustion time, indicating that the diffusion process is dependent on the pollutant concentration. The experimental results show that the steepness of breakthrough curve is intensified by any increase in the flow rate of CR solution. Also, our results proved that breakthrough time, exhaustion time, uptake capacity and the percent of CR sorbed became higher with the increase of soil column height from 5 to 20 cm. This displacement of the front of sorption with soil column depth can be explained by the different conditions for mass transfer.

P20. Theoretical study of the isomerization mechanisms in the ground state of some push-pull substituted azobenzenes

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Azobenzene (AB) exists in two different forms: trans (EAB) isomer, more stable from the thermodynamic and energetic point of view and cis (ZAB)-azobenzene which is metastable.[1,2] The interconversion between EAB to ZAB isomers can be achieved under UV light irradiation and the recovery to the initial form occurs both by visible light irradiation and thermally in dark.[3,4] It is accepted that the isomerization process of azobenzene chromophores can be realized through four mechanisms: rotation, inversion, concerted inversion and inversion-assisted rotation, which are not yet fully elucidated. This study has been proposed to analyze the static mechanism of isomerization during the process of interconversion of azobenzene and substituted azobenzene derivatives, taking into account the group nature from substituents by push-pull effects in different orientations.

The mechanism of isomerization of azobenzene and substituted azobenzenes was developed by theoretical calculations based on DFT (Density Functional Theory) procedures. The results of the theoretical investigation have revealed a new type of isomerization mechanism in the ground state of azobenzene chromophores.

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P21. Gas chromatography-mass spectrometry analysis of intermediates involved in lysergic acid biosynthesis in plants

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Ergot alkaloids are assigned as important therapy and experimental pharmacology relevant secondary metabolites synthesized not directly by plants but usually by symbiotic fungi living on the plants. More than 40 different ergot alkaloids, known also as mycotoxins, are presently known.[1] In the present work, agroclavine, belonging to the group of ergot alkaloids (i.e. ergotamine), has been identified by gas chromatography-mass spectrometry technique in an *Ipomoea tricolor* matrix. Experimental investigations have been undertaken on a commercial available seed collection. Details on preparative and analyses steps are elsewhere presented.[2] The HP-5ms Agilent capillary column used in the present work has been proved to provide similar behavior as that of the previously used DB-5msUI column. Phenols, sugars, squalenes, tocopherols, sterols and agroclavine appear to be among the most important constituents in *Ipomoea tricolor*. Agroclavine is assigned as an important intermediate in the biosynthesis of lysergic acid,[1] a process whose importance might be directly correlated with plant skeleton constituents (leaves, flowers, seeds). Our results might have important implications in the elucidation of the formation pathways of lysergic acid-derived ergot alkaloids produced by fungi from agroclavine alkaloid.

Acknowledgements:
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P24. Complexation of anthracene-imidazolium salt with different acetate ions: UV-vis and fluorescence studies

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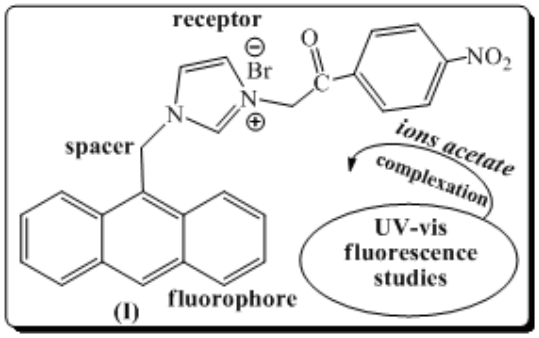
The development of fluorescent receptors for a specific task is of enormous interest in the field of host–guest chemistry, due to their biological and environmental significance.[1-3] In general, most of these receptors consist of imidazolium, benzimidazoliumm or pyridinium units, attached to a fluorophore, which is the anthracene moiety.[1-4]

In this research, our main objective was the synthesis of a new anthracene imidazolium salt with *p*-nitro-phenacyl moiety (I), and to study their complexation ability with different acetate ions. The synthesis was conducted in two steps: *N*-alkylation and the quaternization reaction. Thus, it was obtained the desired PET (photoinduced electron transfer), this being a typical fluorophore-spacer-receptor system. We studied the generation of cycloimmonium ylide, *in situ*, from the anthracene imidazolium salt (I), and complexation with different ions (Cd^{2+}, Cu^{2+}, Co^{2+}, Zn^{2+}, Pb^{2+}), using UV-vis and fluorescence measurements. The absorption and emission spectra were recorded on a Schimadzu UV-1800 spectrometer and a Edinburgh Instruments 900 Xe Spectrofluorometer, respectively.



Acknowledgements:
This work was supported by PN-II-DE-PCE-2011-3-0038, no.268/05.10.2011. We also thanks to the POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010 Project, CERNESIM, for fluorescence measurements.

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P26. Synthesis of new peptides with neuroprotection activity and study of affinity for metal ions

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NAP is the smallest active fragment, which was recognized as a neuroprotective moiety of activity-dependent neuroprotective protein (ADNP).[1] This peptide with the sequence Asn-Ala-Pro-Val-Ser-Ile-Pro-Gln is capable of crossing the brain biomembrane barrier and is nontoxic, therefore it is considered an important candidate for future drug development.[2] It was initially used to protect against β amyloid toxicity (because it binds the amino acid residues 25–35) in rat cerebral tissue and later studied for its protection against β amyloid in neuronal enriched cultures.[3, 4]

Our experimental results are focused on the synthesis and characterization of some modified peptides, which could be used as potential therapeutic agents in neurodegenerative diseases like amyotrophic lateral sclerosis and Alzheimer's disease. These were obtained using solid phase peptide synthesis strategy and analyzed by mass spectrometry, NMR and FT-IR spectroscopy. Although FT-IR spectra of peptides are complex and difficult to interpret, these offer useful details for both structural characterization and conformational changes of peptides. Also, Atomic Force Microscopy studies reveals their particular affinity for metal ions.

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P27. Yeast-based microbiological decontamination of heavy metal contaminated soils: Tarnita area case

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This paper projects the potential of active and inactive yeast (Saccharomyces cerevisiae) in biosorbing heavy metals from contaminated soils, originated from a sterile dump. Both living and dead yeast cells can be effective metal accumulators and there is evidence that some biomass-based clean-up processes are economically viable.[1] The sterile dump from Tarnita mine site, Suceava region and soil around it contain increased concentrations of heavy metals such as Cu, Fe, Pb and Zn, that may affect germination and have toxic effects on plants. The seeds of wheat (Triticum aestivum) used as an indicator of toxicity, have interrupted germination when grown on small amounts of polluted soil from the dump, but germinated when the toxic substances were removed by washing heavy metal contaminated soil with water in ratio 1: 10 the soil: water. Toxic metals were concentrated in the first washed supernatant, which was subjected to the yeast-based microbiological decontamination. We investigated the role of active and inactive yeast in the removing of contaminants from toxic supernatants. Decontamination by yeast could be a useful method as it has been extensively studied for the property of retaining heavy metals such as Cd, Co, Cr, Cu, Pb and Zn. Metal remediation by common physico-chemical techniques is expensive and unsuitable in case of low metal contamination.[3] The biosorption experiments using yeast could serve as an economical means of treating effluents charged with toxic metallic ions.

Acknowledgement:
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P28. Synthesis of $NiAl_{2-x}Cr_xO_4$ by sol-gel method using fructose as fuel agent

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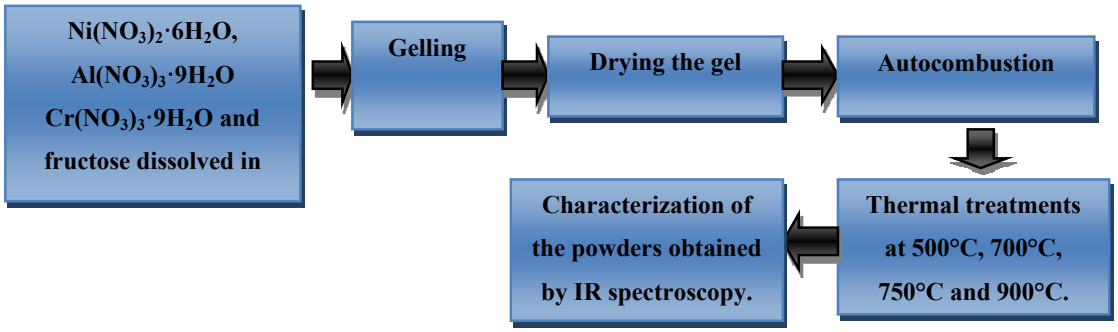
Spinel type compounds have the general formula AB_2O_4, where A is a divalent cation: Ni^{2+}, Zn^{2+}, etc., with a tetrahedral coordination and B is a trivalent cation: Cr^{3+}, Al^{3+}, etc., octahedrally coordinated.[1]

In this work the spinel compounds, double substituted on the B position: $NiAl_{2-x}Cr_xO_4$ (x = 0-2) were synthesized by sol-gel autocombustion method using fructose as complexing/fuel agent. IR absorption spectroscopy was used as a method of following the chemical reaction in the solid phase. In the IR spectra of the samples the characteristic peaks for spinel structure were observed, as well as the disappearance of the organic phase. The fuel agent was characterized by thermal analysis to evaluate the autocombustion temperature.

The nickel chromite ($NiCr_2O_4$) is currently used in the processes like catalysis and oxidative dehydrogenation of propane.[2] Nickel aluminate ($NiAl_2O_4$) is used in the pigmentation of ceramic in the coating and in catalyst.[3]

The synthesis protocol used is presented below:



Acknowledgements:
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P29. Essential elements in forages from permanent grasslands of North-Eastern Romania. Implications for animal nutrition

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The aim of the study was to determine the concentration of a number of essential elements in forages from organic and mineral fertilized permanent grasslands and to relate these concentrations to animal requirements and potential impact on animal performance. Forages were collected in 2010, 2011 and 2012 from four natural permanent pastures with predominant *Nardus stricta* L., *Festuca rubra* L. and/or *Agrostis capillaris* vegetation. The fertilization experiences started in 2006 and different variants of treatments were applied: Cosna – organic and mineral fertilization (9 and 7 variants); Saru-Dornei – organic fertilization (5 variants); Pojorita – organic and (organic + mineral) fertilization (7 and 7 variants); Putna – organic fertilization (5 variants). Freshly harvested samples were dried at room temperature, ground to obtain a homogeneous matrix and analyzed to determine major minerals (Na, Mg, Cl, K, Ca, P) and micro-minerals (Mn, Fe, Co, Cu, Zn, Se, Mo). Essential elements concentrations were compared to the recommended dietary mineral requirements and the maximum tolerable limits for dairy and beef cattle. Most of the samples have concentration in and above the requirement range but not higher than maximum tolerable limit. Only a small percentage of samples and elements have values above the maximum tolerable limit. Sodium concentrations in all samples are bellow requirements. A quite significant part of samples in all experiments, except Pojorita, have a lack of Mo. The calculated values of Dietary Cation-Anion Difference (DCAD) show that all the forages meet the dietary conditions for lactating cows. Forages in all experiments, except one, with exclusive or mixt (organic + mineral) fertilization have higher DCAD values compared to those collected in experiments with mineral fertilization. A t-test was applied to verify that fertilizer supply significantly change the content of essential elements in forages. The results indicate no significant differences in Se concentrations in all samples, Mo in all experiences except Cosna. The most significant differences were found in forages in Cosna experiment, where Cl, K and Ca have quite similar behaviour.

P30. Decolorization of Basic Blue 41 by hydrogen peroxide using a heterogeneous catalytic system consisting of Cu(II)–macroporous chelating polymer functionalized with diethylenetriamine

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The decolorization of the water-soluble cationic dye Basic Blue 41 (BB41), in aqueous solutions with hydrogen peroxide, by using a heterogeneous catalyst (Cu(II)-A) based on Cu(II)-macroporous chelating polymer functionalized with diethylenetriamine (DETA) was investigated. The catalytic capacity of a number of products resulting from the saturation of some weak basic synthesized chelating resins with the metallic ions Cu(II), Co(II), Ni(II) was initially tested in the process of BB41 decolorization with H_2O_2 and it was noticed that Cu(II)-A is the most effective catalyst. The decolorization efficiency was found to depend on: initial pH of the solution, H_2O_2 concentration, dye concentration, reaction time, amount of catalyst and temperature. In order to find the optimum pH for the decolorization of BB41, a series of experiments were conducted at different pH values in the range 3 - 12 and the results indicate the most efficient decolorization at pH 8. The effect of H_2O_2 concentration at the optimum pH (8) was studied in the range from 50 to 470 mmol L^{-1}. Significant decolorization (85%) occurs even at small concentrations (50 mmol L^{-1}), in 30 min. Increasing the concentration of H_2O_2 leads to an increase in the decolorization efficiency and a constant level is reached in the range 150 – 470 mmol L^{-1} H_2O_2. Batch experiments with dye solution at 150 mg L^{-1} dye solution (pH 8, H_2O_2 concentration 370 mmol L^{-1}, 0.06 g catalyst) showed the almost complete decolorization (after 60 minutes) at a temperature of 22 ºC and complete dye decolorization after 10 min at 50 ºC. The oxidation reaction exhibits first-order kinetics with respect to dye concentration. The activation parameters, such as activation energy, activation enthalpy and entropy were also calculated by using the Arrhenius and Eyring equations. The tested catalyst has a good stability (1-2 % metallic ion released in the solution) and is efficient for the decolorization of BB41 dye in mild reaction conditions.

P31. La(Sm)$Fe_{1-x}Co_xO_3$ perovskite

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$LaFeO_3$ with an orthorhombic phase of the ABO_3-type perovskite structure has become a currently attractive research topic because it is proposed for various applications in several advanced technologies such as catalysts[1] various kinds of chemical and gas sensors and electrode materials in solid oxide fuel cells.[2]

La(Sm)$Fe_{1-x}Co_xO_3$ (where x =0; 0,05; 0,1; 0,2; 0,3) perovskite were prepared by the sol–gel auto-combustion method and sintered at 750 °C for 6 hours. The role of La(Sm) cations and the substitution degree (x) on the structures, morphologies and catalytic properties was investigated. The progress of perovskite type structure formation and the disappearance of the organic phases were monitored by infrared absorption spectroscopy (FTIR). Perovskite oxide structures were evaluated using X-ray diffraction (XRD). Also, BET surface areas were measured at the liquid nitrogen temperature by nitrogen adsorption. Catalytic properties of the oxide compounds were evaluated by test reaction of hydrogen peroxide decomposition.

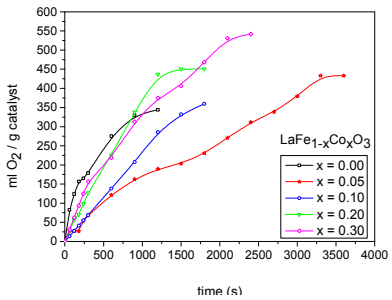

Figure 1. Variation of O_2 quantity with time in presence of $LaFe_{1-x}Co_xO_3$ as catalyst

The XRD samples show an orthorhombic structure for all the sintered samples. The La(Sm)$Fe_{1-x}Co_xO_3$ perovskites exhibit a good catalytic activity for the H_2O_2 decomposition with the rate constants of first order. The higher values of decomposition yields and rate constants were obtained for $LaFe_{1-x}Co_xO_3$ series (Figure 1).

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P33. Functionalized polymers for new applications

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The paper provides information concerning recent advances in functionalized polymer compounds, especially for polysulfones, based on the synthesis process, computerized structures used to evidence specific properties, adaptation of various structures for specific applications, thermodynamic aspects. Are presented some molecular technologies, thermodynamic aspects, obtaining of nano- or bio-materials - involving biocompatibility and antimicrobial properties, formation of metal nanoparticles in polysulfonic matrices, metal film deposition on polysulfone surfaces, polysulfone compounds with chelating groups or specific electro-optical properties, all discussed in the context of possible new applications.[1] Combining different properties of functionalized polysulfones with their technologies for obtaining complex structures for specific applications, the paper demonstrates the importance of these materials in electrotechnic domains, biotechnology, biomedicine, or environmental remediation. Moreover, special applications of functionalized polysulfones, deposition mechanisms of metal nano-particles and nano-layers on modified polysulfones, self-assembly of metal particles on polymeric films, elasto-plastic properties of metal layer/polysulfone complexes, and polysulfone composites characterized by formation of metal nanoparticles in polysulfone matrices or chelating groups in polysulfones for heavy metal retention, are aspects presented in paper.

In addition, it offers recent scientific information and can significantly enrich the basic knowledge of students and researchers working in the field of polymeric materials: physicists, chemists, engineers, bio-engineers, biologists.

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P34. Comparative Theoretical Study of the cyclisation of several symmetric and asymmetric diarylethenes

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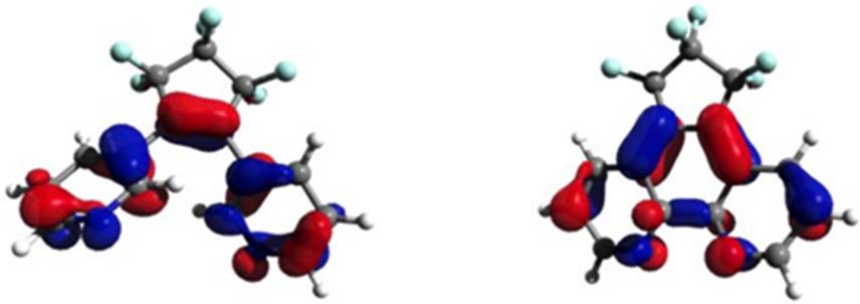
The cyclisation energy of several photochromic perfluorocyclopentenediarylethenes (symmetric, asymmetric, inverted as well as substituted) has been investigated using the time dependent - density functional theory (TD-DFT). Molecular geometries in ground state and theoretical energy for all molecular structures included in this study were computed at the B3LYP hybrid density functional level using the 6-31G(d) basis set, making a compromise between computer resources, time consuming and accuracy of results. All theoretical computations were carried out using the Gaussian 09 suite program on a local computer cluster. Among the systems under investigation, symmetric diarylethenesare found to yield consistently the most stable cycloadducts. Preliminary results are correlated with the topology of the frontier orbitals and supports the (photochemical) cyclisation mechanism.



HOMO orbitals of the an diarylethenes structure

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P35. Synthesis of a functional polymer as porous crosslinked beads containing alicyclic groups, potentially useful as high temperature microcontainers

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A new partial-alicyclic copolyimide (CPI) based on bicyclo [2.2.2] oct-7-ene-2,3,5,6-tetracarboxylic dianhydride (BOCA) was synthetized. This unsaturated polymer was used to prepared a porous crosslinked network in bead form, by using the suspension polymerization method. It was copolymerized with N-(4-carboxy-phenyl)maleimide (CMPI) and ethylene glycol dimethacrylate (EGDMA), respectively, in presence of different porogens containing combinations between 1-methyl-2-pyrrolidone (NMP), benzyl alcohol (BzOH), and *N,N*-Dimethylacetamide (DMAc). The resulting polymer beads morphology, influenced by different factors, together with some characteristics including the specific and apparent densities, porosity, pore volume, surface area were studied. Thermal properties and the swelling tendency in different organic diluents - for some chosen samples - were also determined.

The best polymer beads were obtained in a reaction system with a solubility parameter value δ_{por} =23,59MPa ½ for poly(CPI –co- CPMI) and δ_{por} =23,23 for poly(CPI –co- MEG) respectively, using a crosslinker concentration was of 40 %. The crosslinked beads are thermally stable around of 400ºC, having a pore volume in the range of 0.5÷2.3 mL/g, a surface area in the range of 195÷360 m^2/g and enhanced swelling properties.

The study provide a new approach to synthesis functional porous crosslinked networks in beads shape, starting from an unsaturated copolyimide, in accordance with the principles of the suspension polymerization. The study opens new perspectives to obtain complex systems, with potential functional advantages for high performance applications.

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P36. Synthesis, characterization and toxicity analysis of some Mn(II), Co(II), Ni(II) and Cu(II) complexes with N-(p-nitrobenzoil)-L- glicina

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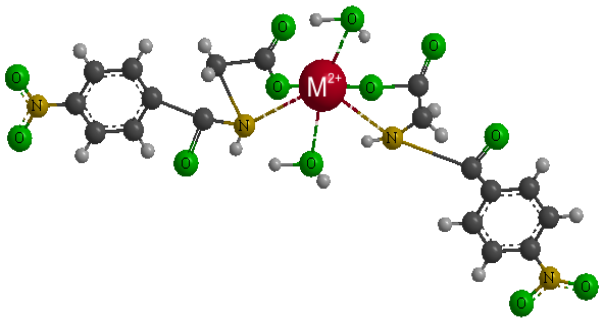
This paper presents the synthesis, structural and physico-chemical characterization of Mn(II), Co(II), Ni(II) and Cu(II) complexes with N-(p-nitrobenzoil)-L- glicina[1] as ligand. Firstly, four complexes were synthesized in 1:2 molar ratio, followed by their characterization and determination of their toxic potential (toxicity lethal dose) as well analysis of some antifungal and antibacterial properties.

In order to determine the structure of the new combination were made following investigations: elemental analysis, FTIR spectroscopy, X-ray diffraction (XRD), electron spin resonance (ESR), UV-Vis absorption spectra, and thermogravimetric analysis. Experimental data shows that all compounds have a crystalline structure framed orthorhombic system and are thermally stable up to temperatures above 100 °C. From the data obtained the compounds shown the following structure.[2]



Toxicity tests of new compounds were run on mice and the results indicate that the lowest value of the lethal dose is displayed by the copper compound. The biological and antifungal activities were investigated for all compounds. The cobalt compound has the best antibacterial properties and the copper compound presents the best antifungal properties.

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P37. Magnetic properties of quaternary ferrites

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Spinel ferrites have proven to be extremely useful materials, with numerous applications in various fields, in electronics in particular.[1] Due to the specificity of the properties required for these materials and their applications, it is of great importance to determine the underlying connections between the nanoparticles' composition, size and morphology with their properties.[2]

Based on this premises M0.25Cu0.25Mg0.5Fe2O4, where M can be Mn, Zn, Co, Ni, ferrite nanoparticles were obtained using the coprecipitation method[3] and were characterized by means of X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and morphologically using scanning electron microscopy (SEM). The presence of organic groups belonging to carboxymethylcellulose (CMC), the surfactant used, was confirmed using infrared spectroscopy (FT-IR), XPS and differential scanning calorimetry (DSC). The magnetic properties were studied using vibrating sample magnetometry (VSM).

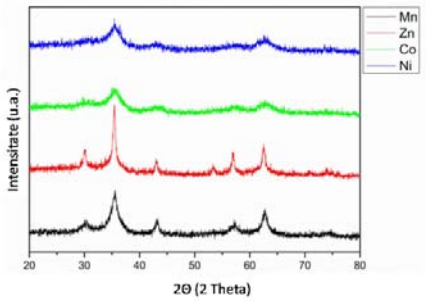

Figure 1. XRD spectra for $M_{0.25}Cu_{0.25}Mg_{0.5}Fe_2O_4$, (M = Mn, Zn, Co, Ni).

Acknowledgement:
The authors wish to thank ANCS Romania for the financial support

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P38. Cytotoxic activity of some dihydroxyacetophenone derivatives

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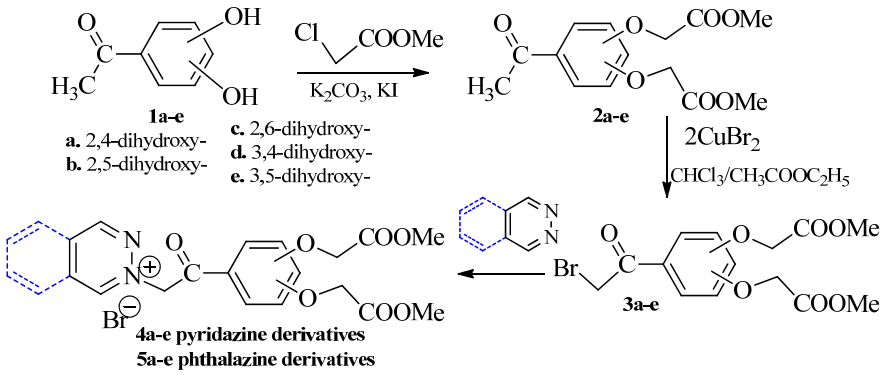
The cancer chemotherapy is complex and complicated, mostly because of the significant levels of toxicity and the emergence of drug resistance and multidrug resistance. It is obvious that development of new chemotherapeutics is of major interest in academic and industrial research, in order to discover newer and more potent molecules, with higher specificity and reduced toxicity than the existing ones. [1-3]

The strategies adopted for the synthesis of our dihydroxyacetophenone derivatives **2-5** involves three steps: *O*-alkylation, α-bromination of dihydroxyacetophenone followed by an *N*-alkylation of 1,2-diazine derivatives, Scheme 1.



The *in vitro* cytotoxicity of the synthesized compounds was evaluated on HeLa cells by the MTT assay according to Mosmann's method. The brominated compounds showed the highest cytotoxicity, these compounds being more active than positive controls.

Acknowledgements:
The author Zbancioc Ana Maria wants to thank to grant **POSDRU/159/1.5/S/137750**, Project "Doctoral and Postdoctoral programs support for increased competitiveness in Exact Sciences research", cofinanced by the European Social Found within the Sectorial Operational Program for financial support.

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P39. Pyridazinones with acetylhydrazine skeleton: synthesis and stereochemical investigations

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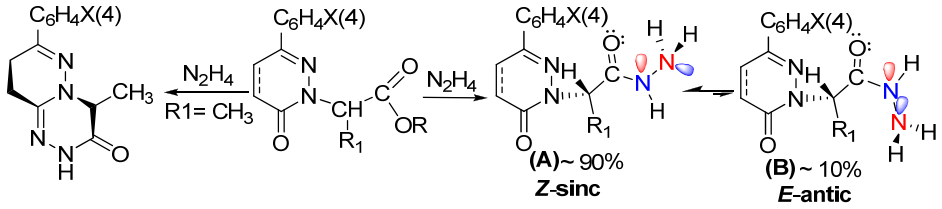
The pyridazine moiety and its 3-oxo-derivatives are considered as privileged structures since they were found to possess a large range of biological activities (antimicrobial, analgesic and anti-inflammatory, cardiovascular and antihypertensive activity) and are used as reactive precursors in the synthesis of many important organic molecules.[1-4]

In the present research work, our main objective was the synthesis of some pyridazinones with acetylhydrazine skeleton and the investigation of the stereochemical aspects, do to the presence of the hydrazide (R-CO-NH-NH_2) moiety (scheme 1).



Scheme 1. Representation of conformational equilibrium and cyclocondensation of the obtained compounds

In order to prove the *Z-sc/E-ac* stereochemistry unequivocally, we performed a NoeDiff 1D experiment, which provides direct evidence in this respect. Also, the structure of the fused obtained heterocycles was proved by X-ray structure measurement.

Acknowledgements:
Dorina Mantu is thankful for the financial support of grant POSDRU/159/1.5/S/133652, co-financed by the European Social Fund within the Sectorial Operational Program Human Resources Development 2007 – 2013 and the POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010 - CERNESIM Project, for NMR experiments.

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P40. An anova study about photocatalytic reactivity of titania thin layers

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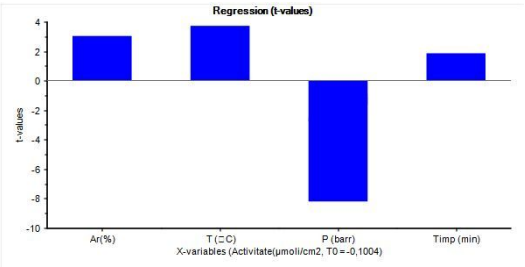
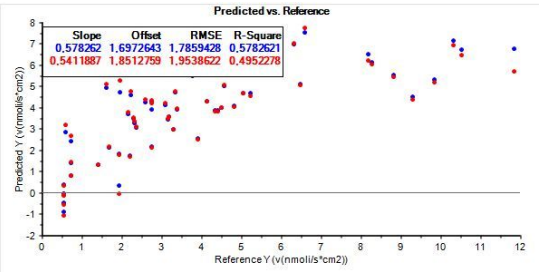
Photocatalysis is an advanced oxidative process occurring on interface photocatalyst/reaction media, when photocatalyst is activated by ultraviolet or visible light. It appears because in a semiconductor under irradiation, electron-hole pairs are created and subsequent, very reactive atomic and molecular species formed on surface are able cu initiate redox reactions. Thin layers of titania were fabricated by sputtering method using a DC magnetron. The photocatalytic activity of the layers was determined in a self-conception reactor by the capability to degrade gaseous formaldehyde. This study used MLR (multilinear regression) for statistical analysis of data, because the great number of experiments lends an Anova study. Unscrambler X software was the computing instrument. The level *p* of statistical significance and *F* ratio were the parameters used to find correlation between entry-parameters and out-parameters. The considered entry-parameters were pressure, temperature of substrate, argon concentration and time of sputtering, all of them measured during the active process of sputtering. The out-parameters were the global reaction rate of redox reaction occurred on photocatalyst surface and a maximum rate calculated by fitting curves analysis method.



Regression (values in the ANOVA) for the maximum reaction rate calculated by the inflection point of the logistic curve of the thin titanium dioxide layer on the deposition parameters



The predicted values to the reference speed calculated by the reaction of the inflection point of the logistic curve of the titanium dioxide layers on the deposition parameters

P41. Environmental impacts evaluation of polyhydroxyalkanoates (PHAs) with recipe method

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Biopolymers as polyhydroxyalkanoates (PHAs) are considered sustainable polymers produced from recoverable resources. Their utilization represents a viable solution for solving the relevant environmental impacts generated by synthetic polymers, as a result of a high consumption of crude oil, considered an expensive, nonrenewable and scarce resource. In this paper, we have analyzed a biotechnological production process of polyhydroxyalkanoates (PHAs), using organic waste as raw materials. We performed the environmental evaluation of the PHAs production using Life Cycle Assessment (LCA) tool, in particular ReCiPe method. The functional unit chosen was 1 kg PHAs. For the each stage included in production process, the inputs and outputs were established. The impact categories considered in our evaluation were as follows: *climate change human health* (CcHh); *human toxicity* (HT); *terrestrial acidification* (TA); *photochemical oxidant formation* (POF); *freshwater ecotoxicity* (FE); *marine ecotoxicity* (ME). Results showed positive values for all impact categories associated to PHA production, meaning negative impacts on the environment, their magnitude decreasing in the following order: CcHh>HT for human impact (Figure 1a), and TA>POF>FE>ME for environmental impact (Figure 1b). These impacts are however less significant compared with those resulted during synthetic polymers production.

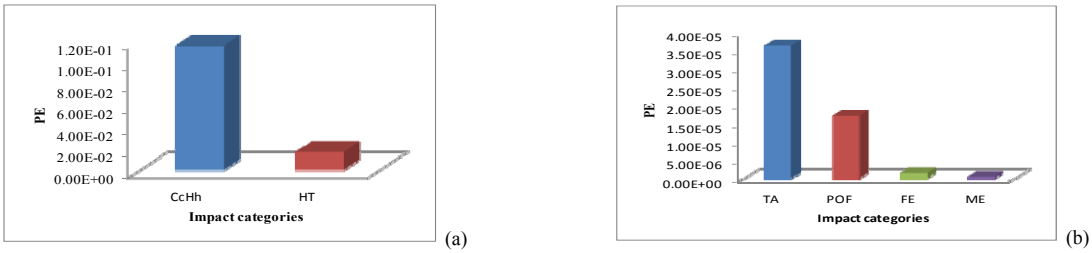

Figure 1. Environmental impacts using ReCiPe method resulting in the production of PHA process: (a) human impact; (b) environment impact

Acknowledgment:
This work was supported by the grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project number PN-II-ID-PCE-2011-3-0559, Contract 265/2011, GaBi Education: Software and database for Life Cycle Engineering, PE INTERNATIONAL GmbH and by the strategic grant POSDRU/159/1.5/S/133652, co-financed by the European Social Fund within the Sectorial Operational Program Human Resources Development 2007 – 2013.

P42. Evaluation of municipal solid waste scenarios with AHP and electre techniques

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Effective disposing and recycling of solid waste has become mandatory due to the continuous increase of environmental problems generated by solid waste generation and regulatory constraints. In this framework, modelling of municipal solid waste management (MSWM) area by applying multicriteria analysis is an efficient and advanced scientific support for decision-makers in the selection of the most suitable MSWM system for implementation. In our study, we elaborated four MSWM scenarios for Iasi city (S1 – S4) (Fig. 1), including the following specific unit operations: temporary storage of waste in containers (TS); collection and transport (CT); treatment/elimination by sorting (S), landfilling (L), composting (C), incineration (I). The scenarios were evaluated in terms of sustainability by two multicriteria analysis methods: *Analytic Network* in the form of *Analytic Hierarchy Process* (AHP) and *Elimination et Choice Translating Reality* (ELECTRE). The evaluation of MSWM scenarios illustrated in Figure 1 is based on economic, environmental and technical criteria (costs, benefits, climate change, eutrophication potential, energy consumption etc.). AHP was used to divide a decision problem into a set of clusters and sub-clusters by ranking components into a hierarchical structure similar to a family tree. Application of ELECTRE involved the construction of the evaluation matrix, calculation of the outranking relation and exploitation of the outranking relation. Results showed that the scenarios S3, S2 have a good score in terms of their sustainability, while S4 and S1 show extremely weak performances, being completely unfavorable for application.

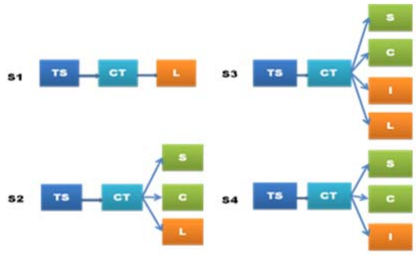

Figure 1. MSWM scenarios evaluated

Acknowledgment:
This work was supported by the grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project number PN-II-ID-PCE-2011-3-0559, Contract 265/2011 and by the strategic grant POSDRU/159/1.5/S/133652, co-financed by the European Social Fund within the Sectorial Operational Program Human Resources Development 2007 – 2013.

P43. 5D cyanido complex as building block for magnetic materials

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Over the last two decades, low-dimensional magnetic systems have been a core interest in the field of molecular magnetism. In particular, molecular complexes such as Single-Molecule Magnets (SMMs) and one-dimensional solids such as Single-Chain Magnets (SCMs) have been a topic of intense research activity. Of special interest is their slow magnetization dynamics, which give rise to magnet-like behavior at the molecular level. Heterobimetallic coordination compounds featuring various transition metal ions have significantly enriched our understanding of SCM properties. In the design of such systems, molecular building units bearing bidentate ligands such as cyanide groups (CN^-) have been extensively employed. Besides the catalogue of well known hexacyanidometallates, chemists are particularly interested in mononuclear *trans*-cyanide transition metal complexes to build one-dimensional heterometallic compounds, mainly because the cyanide moiety allows a highly directional coordination mode and behaves as a good mediator of magnetic exchange between spin carriers.

Recently have been reported the highly anisotropic building unit *trans*-$[Re^{IV}Cl_4(CN)_2]^{2-}$ with a spin ground state of S = 3/2, which can form SCMs with 3d transition metal ions (Mn^{II},Mn^{III}, Fe^{II}, Co^{II} , Ni^{II})[1]. In order to further explore these bimetallic 3d-5d systems, we report our studies on $[Re^{IV}Cl_4(CN)_2]^{2-}$ linked to anisotropic building-block based on N1,N4-bis(salicylidene)S-alkyl-isothiosemicarbazide manganese(III) Schiff base to design 1D system (Figure 1), which exhibits SCMs behavior.

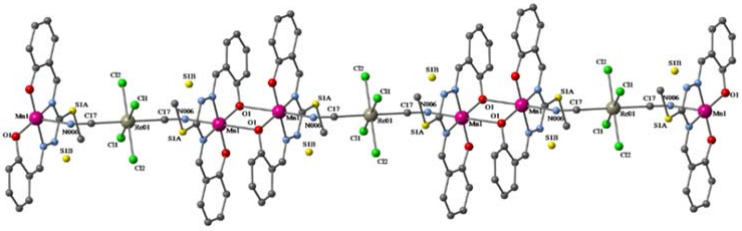

Figure 1. Crystal structure of 1D system $[\{Mn^{III}(L)\}_2\{Re^{IV}Cl_4(CN)_2\}]$

References:

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P44. Synthesis, characterization and biological investigation of copper(II) complexes with 4-methylthiosemicarbazone 8-formylquinoline

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Thiosemicarbazones and their metal coordination compounds are a broad class of biologically active products which show antifungal, antibacterial, anti-inflammatory, antiviral and antitumor activities.[1,2] The interest of cooper(II) coordination compounds with 8-formylquinoline thiosemicarbazone derivatives has been increased because their biological activities are often enhanced on complexation.[3] In this work we report the syntheses, structures and characterization of copper(II) coordination compounds with 8-formylquinoline 4-metylthiosemicarbazone (HL) containing acetate (**1**) and chloroacetate (**2**) anoin. The HL ligand was obtained by refluxing in ethanolic solution 8-formylquinoline and 4-metylthiosemicarbazide. The compound were synthesized by reacting the ligand with copper(II) salts in 1:1 molar ratio in ethanolic solution.

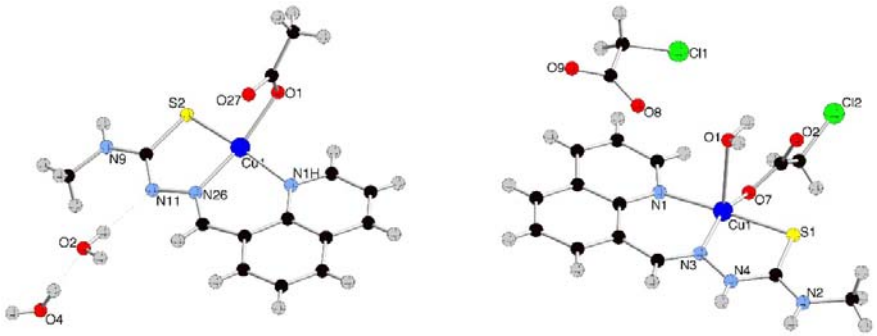

Figure 1. Crystal structure of the compound **1** and (2)

Biologic investigations show that this compounds can be used as inhibitors for the biosynthesis of proteolytic enzymes with the aim to stabilize the composition of enzyme complexes.

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P45. Synthesis and structure of copper (II) complex with 5-sulfosalicylaldehyde thiosemicarbazone

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The thiosemicarbazone-based ligands have an important role for compounds with chemical, analytical, catalytic and biologic properties. On the other hand the thiosemicarbazones based compounds show low solubility in water. This problem can be solved by functionalization of coordinating ligands with easily ionizable groups. In this context, it was carried out the synthesis of copper (II) coordination compound with 5-sulfosalicylaldehyde thiosemicarbazone (5-SO_3TSCAS) ligand. The ligand (5-SO_3TSCAS) was obtained by refluxing of 5-sulfosalicylaldehyde sodium salts and thiosemicarbazide in 1:1 molar ration in aqueous ethanol. The interaction of the investigated 5-sulfosalicylaldehyde thiosemicarbazone with copper (II) salts in water allows the formation of green crystalline product (Figure 1).

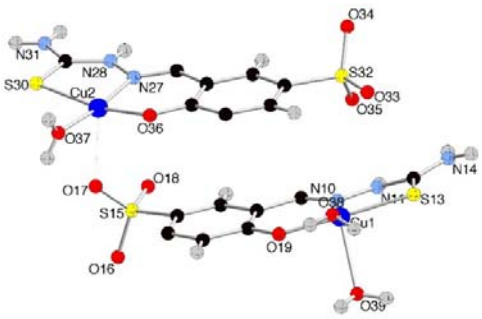

Figure 1. Crystal structure of $[CuL\cdot H_2O][CuL\cdot 2H_2O]$.

The study of the crystal structures of obtained compounds shows that the anions do not have influence on the coordination mode. The molecular structure represents a dimer assembled by coordination of one oxygen atom from the sulfonate group of the neighboring unit. All copper (II) ions are in pyramidal geometry: Cu1 is coordinated to the ligand via ONS donor atoms and two water molecules; Cu2 is coordinated to the ligand via ONS donor atoms, one water molecule and O17 from neighboring sulfonate group. The obtained product $[CuL\cdot H_2O][CuL\cdot 2H_2O]$ is perfectly soluble in water and its biologic studies are in process.

P46. Prediction of best-fitting isotherm model by comparing error criteria in linear and non-linear regression analysis of hazardous heavy metal adsorption onto functionalized polymers

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In an adsorption system, the equilibrium state is characterized by the relationship between the amount of adsorbate adsorbed and the amount of adsorbate remaining in solution. The experimental equilibrium isotherm expressing the change with increasing adsorbate amount in solution of adsorbate distribution between the solid and liquid phases may be analyzed by various equilibrium isotherm models to determine the model which provides the best mathematical description. It is important to find the best-fitting model since the implied thermodynamic assumptions and parameter estimates offer information that are necessary for optimizing the design of the adsorption system, e.g., adsorbent surface properties, adsorbent-adsorbate affinity and adsorption mechanism.

In the present study, linear and nonlinear regression analysis methods are employed to analyze various isotherm models in order to establish which one offers the best fit of the experimental equilibrium data for the adsorption of some toxic metal ions from aqueous solutions onto crosslinked polystyrene beads functionalized with ionic liquid-like moieties. To reliably assess the applicability of equilibrium isotherm models for the studied adsorption systems, i.e., the goodness of fit between the adsorption capacities experimentally determined and those predicted by the model, nine error functions, which are either relative or absolute, were employed: the adjusted coefficient of determination, the average relative error, the sum of the absolute errors, the average absolute error, the root mean square error, the average relative standard error, the chi-square test, the hybrid fractional error function and the Marquardt's percent standard deviation. The results of isotherm modeling are consistent with chemisorption occurring in the studied adsorption systems. The regression analysis method (linear or nonlinear) which provides the best fit of the experimental data depends on the equilibrium isotherm model considered.

P47. Equilibrium isotherm studies on removal of toxic metal ions from aqueous solutions by non-porous polymeric adsorbents

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Heavy metals have a high toxicity making a great impact on environment quality and human health, therefore their removal from contaminated waters is an absolute necessity. In this study, the adsorption of some heavy metal ions from aqueous solutions onto functionalized polymer beads in single component systems was investigated and the equilibrium isotherms determined. The polymer beads are non-porous, as revealed by the investigation of their surface morphology using scanning electron microscopy and atomic force microscopy; since the diffusion of adsorbate species inside the adsorbent beads is not possible, the functional groups involved in the adsorption are only those located on the bead surface. Adsorption studies were carried in batch mode by varying the initial metal ion concentration and pH value. The experimental equilibrium results were analyzed using several two-parameter isotherm models. In order to determine the best fit isotherm model for each adsorption system, the coefficient of determination was used as criterium of model applicability. The values of this error function indicated that the equation providing the best description for the sets of experimental results depends on the metal ion species. The ranking of isotherm models by ability to simulate the experimental results was established. Among the models studied, Langmuir and Temkin equations are the most suitable to satisfactorily describe the equilibrium data, whereas Freundlich model provides the poorest fit. The isotherm modeling results show that the adsorption of metal ions onto the functionalized polymer surface is a monolayer process, the adsorption sites are energetically equivalent and no lateral interaction takes place among the adsorbed species. The maximum adsorption capacities were calculated from the Langmuir model. The values of the thermodynamic parameters reveal the feasibility and the spontaneous nature of the adsorption process.

P48. Pure and doped TiO_2 thin films for environmental and energy applications

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Pure and doped TiO_2 thin films were grown onto Corning 1737F glass and silicon substrates in by magnetron sputtering in different growth conditions. Structural investigations carried out by X-ray Diffraction showed that films are amorphous and Atomic Force Microscopy (AFM) characterization showed a strong influence of growth parameters on the film surface properties such as the film roughness, the grain shape and dimensions. UV-VIS transmittance versus thickness and hydrophobic to hydrophilic transition under UV exposure were also studied as a function of growth parameters. The results prove the possibility of surface engineering via growth for the achievement of specific metal oxide film application. Very good TiO_2 thin films for both, energy and environmental applications were obtained using one of the most suitable large area growth techniques.

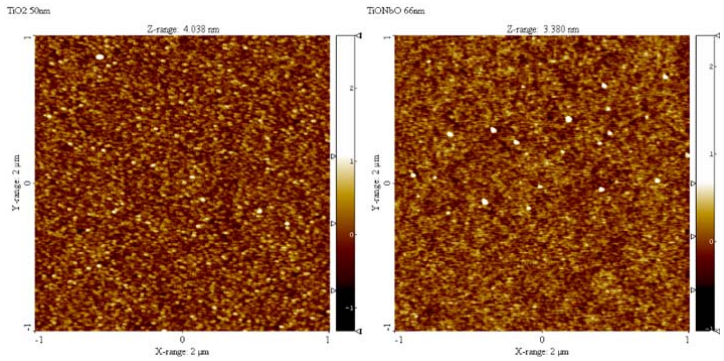

Figure 1. AFM images of pure and Nb doped TiO_2 films a) 50 nm pure b) 66 nm doped. Scan size 2x2µm.

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