International Conference

PROCESSES IN
ISOTOPES AND MOLECULES

Cluj-Napoca 2011

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Welcome at PIM'11

It is a pleasure of National Institute for Research and Development of Isotopic and Molecular Technologies to host the International Conference Processes in Isotopes and Molecules (PIM).

The PIM conference, started in 1999 as a local event, is now an international conference organized every two years by our institute in Cluj-Napoca, the capital city of Transylvania, Romania.

The meetings are attended by researchers in the field of atomic and molecular physics, those developing new materials and technologies, as well as researches in stable isotopes field. The scientific subjects are at the cross-roads of three fundamental research areas: physics, chemistry and biology.

Topics:

T1 - Molecular, biomolecular and environmental systems

T2 - Advanced technologies, applied research

T3 - Nanostructured materials and nanocomposites

T4 - Isotopic materials and processes

Note: The contributions to PIM are labeled using the format *Ti-j*, where *i* denotes one of the above topics and *j* denotes the contribution identification. Please follow this rule to track your contribution(s) in this *Book of Abstracts* or elsewhere.

ABSTRACTS

Plenary Pl-1

Stacking of Pie-Slices,- A Chemical Nanotechnology ?

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Abstract. In the frame of this presentation 'Chemical Technology' is defined as the approach to optimize technical procedures by exploiting the chemical, and physical properties of the involved compounds. ‘Organogels’ are elastic- or viscoelastic materials consisting of organic solvents and low molecular weight organic ‘gelators’. The gelator forms three-dimensional networks of supramolecular structures confining the solvent. Very efficient gelation is found with gelator molecules that self-assemble to fibrous structures of large aspect ratios, e.g. rods or ribbons. With the example of supramolecular organogels it is demonstrated how organic chemists may apply simple heuristic rules to design fibrillar nanostructures. Molecular designed fibrillar superstructures offer the possibility to generate molecular systems that selectively transport electrons, photons, ions, or molecules, and can be used as the basis to generate functional materials such as thermo-, and mechano reversible gels, ion-selective membranes, or metallized organogels.

Plenary Pl-2

Nanofluidics in carbon nanotubes

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Abstract. Novel results, obtained by molecular dynamics simulations, concerning the ionic transport in aqueous solutions through carbon nanotubes are presented. Specifically, the effects of the nanotube radius, solute concentration, and applied external electric fields on the solution structuring are investigated in terms of spatial density distributions, pair distribution functions, and detailed electrostatics. The structural features are consistent with general theoretical results of nanofluidics (like, for instance, the Donnan-type voltages established at the channel apertures depending on the logarithm of the maximum ion concentration). The transport properties are characterized by mobilities, currents, and pairing times of the solute ions and corroborate, equally, general nanofluidics results (the linear log-log regime of the nanochannel conductance as function of the solute concentration and the current-voltage curve of the channel). Discontinuities in the partial ionic currents are explained on the basis of a recent theoretical model of quantized ionic conductance in nanopores. Correlations between the structural and dynamic properties are established, linking causally the highly structured spatial density profiles, the ion pairing phenomenon and the ionic currents. The simulated properties are based on averages over the largest data collection times reported in the literature (0.8 μs), providing unsurpassed accuracy.

Plenary Pl-3

Carbon nanomaterials for applications in energy, advanced materials, aviation, medicine and agriculture

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Abstract. Given their unique optical, mechanical, chemical, and electrical properties, carbon nanomaterials represent a family of nanoscaled structures that had been intensively studied lately. This interest is explained by their huge potential as multifunctional components in a large number of applications ranging from composites with improved properties, energy generation and storage, aeronautics, medicine, biology, or agriculture. Several classes of carbon nanostructures have been identified: fullerenes, nanotubes and nanofibers, graphitic layers (graphenes), nano-diamonds. Although the fullerenes, nanotubes and the graphenes have a graphitic structure, their properties are significantly different and are based on their dimensional and morphological characteristics and the arrangement of the carbon atoms. As a result, carbon nanostructures have become some of the most considerable multifunctional materials, with high scientific as well as economic potential.

Plenary Pl-4

Curiosities in the universal theory of the separation column

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Abstract. Working in the area of isotope separation, I have developed over years an abstract and universal theory of the separation column. The theory is abstract, as the separation process is generalised, the concrete features being substituted by postulates. It is universal, that is, applicable to any separation process.

The novel approach of the column theory has encountered many peculiarities. In this paper it is shown a series of mathematical curiosities as non-Hilbertian spaces and special range completeness of some sets of proper functions. Also, the power of the universal theory is illustrate by new applications to some complex processes as multicomponent thermodiffusion and thermo-reaction column.

Plenary Pl-5

Interogation of single – molecule chemistry with protein nanopores

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Abstract. Efficient quantification of interactions between protein pores and biological molecules remains an open question in the fields of physical chemistry and pharmaceutics. Among others, single protein nanopores have long been used to detect a wide range of analytes. In this work we review the previous findings of our lab on single-molecule investigation of reversible interactions between various antibiotics and γ-cyclodextrins, through monitoring of ionic current signatures across a α-haemolysin protein entrapping a γ -cyclodextrin molecule. We show how a protein pore-based system as described above permits the detection of, and differentiation among different antibiotics from the β-lactam family. Our data reveal that electric and electro-osmotic driving forces alter the reversible reaction rates of antibiotics interaction with γ -cyclodextrins, as well as free energy changes accompanying the interaction. In a different approach, the wild-type α-haemolysin was employed as a protein nanoreactor in which alterations of the electrical current through a protein containing a lumen-residing, aryl-capped antimicrobial peptide were recorded and studied at the single-molecule level. Energy and steric considerations support the paradigm according to which Met-aryl interactions between aromatic residues placed at a peptide's extremities and methionines forming the α-hemolysin constriction zone may be essential factors for peptide stabilization within the pore lumen, and of particular relevance to the peptide-α-hemolysin interaction.

Plenary Pl-6

Imaging electronic transport inside nanodevices

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Abstract. We use an atomic force microscopy (AFM) based technique to study the electron dynamics inside nanoelectronic systems covered with an insulating layer. This method, called scanning gate microscopy (SGM), consists of using a polarized AFM tip as a flying gate to locally change the electrostatic potential seen by electrons inside the sample, and to record changes of device resistance. The resistance maps obtained with this technique decrypt local electronic properties that are normally averaged in traditional macroscopic measurements. In this talk I will present an overview of our results in this domain.

We study quantum rings (QRs) patterned from a high-mobility InGaAs/InAlAs heterostucture. SGM imaging at low temperature (down to 100 mK) revealed a wealth of features related to the coherent and ballistic electron dynamics inside the confined structure. By comparing such results with quantum mechanical simulations of the local density of states, we concluded that SGM allows to image the electron probability density inside nanodevices.

We also probe the electronic properties of nanodevices in the quantum Hall regime. Recent results demonstrate the ability of SGM to reveal the spatial structure of quantum Hall transport inside a QR and to identify precise locations of confined electron orbits within the device.

Plenary Pl-7

Engineered nanopores for protein detection

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Abstract. A nanopore may act as an amazingly versatile single-molecule probe that can be employed to reveal several important features of nucleic acids and proteins. The underlying principle of nanopore probe techniques is simple: the application of a voltage bias across an electrically insulated membrane enables the measurement of a tiny picoamp-scale transmembrane current through a single hole of nanometer size, called a nanopore. Each molecule, translocating through the nanopore, produces a distinctive current blockade, the nature of which depends on its biophysical properties as well as the molecule-nanopore interaction. Such an approach proves to be quite powerful, because single small molecules and biopolymers are examined at very high spatial and temporal resolutions. I will discuss our recent work that provided a mechanistic understanding of the forces that drive protein translocation through a nanopore. These measurements facilitate the detection and exploration of the conformational fluctuations of single molecules and the energetic requirements for their transition from one state to another.

I will also describe our recent strategies for engineering new functional nanopores, in organic and silicon-based materials, with properties that are not encountered in nature.

Plenary Pl-8

Characterization of Advanced Materials by X-Ray Spectroscopic Techniques

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Abstract. Many new techniques require “advanced materials” with “tailored properties” for specific applications. Such tailoring of material properties can only be achieved from a deep understanding of the electronic structure of the materials in theory and experiment, from bulk to “nano”-dimensions. Powerful methods for the characterization of advanced materials are available in form of different X-ray spectroscopies, which will be briefly described. Since all electronic states can be probed, core levels, valence bands and conduction bands, the orbital ordering as well as element-specific magnetic properties and band gaps can be determined, even phase changes can be observed. In combination with theoretical calculations, an almost complete description of the properties of new interesting materials can be obtained, what will be demonstrated on selected samples, exhibiting high-k-, colossal magneto resistance- (CMR), multiferroic-, spintronic- or super conducting properties.

Plenary Pl-9

Probing protein quaternary structure in live cells

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Abstract. When an optically excited molecule, called a 'donor,' is located within 10 nanometers of an unexcited molecule, part of the donor's energy may be transferred to the second molecule (called an 'acceptor'). This effect, known as Förster (or Fluorescence) Resonance Energy Transfer (FRET), causes the acceptor molecule to emit light with red-shifted wavelengths compared to the excitation wavelength. Detection of such spectral shifts helps determine whether two fluorescent molecules interact with one another. This talk will review the main advances in FRET theory and technology that led to the recent development of FRET into a method for determination of the quaternary structure of protein complexes in living cells. The presentation will begin by identifying the main requirements that quantitative FRET technology for *in vivo* investigations should meet. Then, our pixel-level FRET method will be described, which relies on a novel two-photon microscope with spectral resolution (called an Optical Micro-spectroscopic System, or OptiMiS) and a simple theory of FRET in oligomeric complexes of arbitrary geometry to determine the association stoichiometry and structure of protein complexes in living cells. The talk will conclude with an overview of the results obtained from *in vivo* studies of oligomeric complexes of several membrane receptors and transporters.

Plenary Pl-10

How to store and prepare highly saline waters prior to H and O isotope analyses? – two methodological studies

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Abstract. Safe storage of water samples between sampling and their stable hydrogen and oxygen isotope analyses (determination of δ^2H and δ^{18}O values) is still a topic of concern in hydrological studies. Water sorption and the diffusive transfer of water molecules through organic polymeric material may entail an isotopic fractionation. Furthermore, the determination of δ^2H and δ^{18}O in small aliquots (typically < 5 mL) of saline solutions (NaCl and $CaCl_2$) is known to be difficult due to the hygroscopic behaviour of some salts (especially those involving divalent cations) and their isotopic fractionation effect. In this communication we present the results of two recent methodological studies. 1) The variation of δ^2H and δ^{18}O values of the same water stored in different type of bottles of different organic polymers (plastic), including low and high density polyethylene (LDPE and HDPE), polypropylene (PP), polycarbonate (PC, polyethylene terephthalate (PET), and high resistance Teflon® (PFA) from different size (10 to 500 mL) and wall thickness (0.20 to 1.50 mm), and over a period of time ranging from 0 to 659 days were compared with those stored in bottles of amber glass. In te second methodological study, synthetic salt (NaCl, $CaCl_2$, Na_2SO_4 and NaF) solutions were prepared at different concentrations (0 to near saturation) with five waters of known isotopic composition ($\delta^2H = -275.6$ to 3.4 ‰, $\delta^{18}O = -35.3$ to 0.4‰). Two distillation procedures were tested, and an anion exchange procedure has been developed.

Plenary Pl-11

Carbon-based nanocomposite porous materials for hydrogen storage

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Abstract. Despite intense research efforts, hydrogen storage remains the main challenge for the development of H_2-powered vehicles. As a viable solution may be associated with reversible storage in solid materials, much attention has been given to nanoporous carbons that offer a versatile platform for developing a wide range of variants and composites. Indeed enhanced hydrogen storage capacities have been measured after metal decoration (e.g. Pd, Pt) of porous carbons and the phenomenon has been described by the so-called "spillover" mechanism. On the other hand, nano-confinement within the pore system of carbon matrices has recently emerged as a promising pathway that can alleviate the unfavourable thermodynamic properties of hydrides. This work summarises the main results obtained so far from our studies on the synthesis and performance assessment of such types of composites. Different nanoporous carbon substrates (carbogenic foam, ordered mesoporous carbons, carbon cones) have been prepared, functionalised and doped with metal/alloy nanoparticles to generate composites that revealed remarkably high sorption capacities at room temperature and moderate pressure. In parallel, porous carbons have also been used as hosts of boranate nanoparticles leading to noticeable improvement of their thermal decomposition properties.

Plenary Pl-12

Restoration of water, soil and sewage sludge contaminated by Fukushima nuclear accident

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Abstract. Fukushima nuclear accident took place by tsunami caused by the Great East Japan Earthquake at March 11, 2011. About 15,000 TBq of radioactive substances was released to the atmosphere by the hydrogen explosions of four reactor buildings. These radioactive substances fell down on mountain forest, agricultural land and urban area surrounding the nuclear reactor site. In this lecture, the sequence of the Fukushima nuclear accident and the present situations of three troubled reactors are explained and two pollution clean-up technologies,

(1) Recovery of radioactive Cs from polluted water by the coagulative precipitation technique using ferric ferrocyanide powder (Prussian blue) and an inorganic coagulant (Ion-Reaction N)

(2) Recovery of radioactive Cs from polluted sewage sludge and soil by the combination of the hydrolysis under high temperature and high pressure and the coagulative precipitation using Prussian Blue and the inorganic coagulant.

which have been developed in Tokyo Institute of Technology, are introduced.

Plenary Pl-13

Graphene: from nanostructures to large area sheets

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Abstract. Graphene is the first experimentally isolated two-dimensional crystal. Its unique electronic properties stem from the linearly dispersing electronic bands near the Fermi level, implying that the effective mass of its charge carriers is vanishing. Moreover, the mobility of the charge carriers in graphene is orders of magnitude higher than in silicon. This, combined with excellent thermal conductivity and outstanding mechanical properties, holds the promise of faster and more power-efficient electronic devices. However in its original form graphene is a zero gap semiconductor, therefore it is not directly suitable for digital electronics. Engineering a band gap in graphene is one of the fundamental challenges in graphene research today. A straightforward way to achieve this is fabricating narrow graphene nanoribbons. However, both the width and the crystallographic orientation of these ribbons have to be controlled with almost atomic precision. Here we present two nanofabrication methods developed by us, which are able to fulfil these requirements: (1) Scanning Tunnelling Lithography, which is the most precise nanofabrication technique of graphene developed so far, and (2) Carbothermal etching, based on a selective etching process able to provide atomically smooth edges. Furthermore, real world applications also require high quality, large area (cm^2) graphene samples. A recently developed CVD growth method using copper substrates holds the promise for this realization. We have characterized the structure and electronic properties of large area CVD grown samples employing local probe methods. Here, we present a detailed analysis on their [polycrystalline] structure as well as reveal the role of the grain boundaries in the electronic properties of CVD graphene.

Plenary Pl-14

Coherent spin and charge transport in single crystal magnetic tunnel junctions

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Abstract. The spin polarized transport in magnetic tunnel junctions (MTJ) represents the core of the spintronics, research area with huge integration potential in sensors and new generation of nonvolatile data storage devices. In single crystal MTJs, the electronic transport is strongly dependent on the band structure of the materials, the electrons being described by Bloch wave functions having the symmetries of the crystal. The tunnelling transport is not only dependent on the electron spin but also on the symmetry of the propagating wave function. Novel effects appear, related to the symmetry dependent tunnelling attenuation rates or quantum confinement in skilfully engineered symmetry dependent quantum wells. Our analysis is performed on model MTJs elaborated by Molecular Beam Epitaxy and/or sputtering. Micrometric size MTJ devices are patterned by UV lithography and ion etching. Two regimes are investigated. In the low barrier thickness regime (below 4 monolayers), the spin currents determine by spin torque effects an antiferromagnetic coupling. In the larger barrier thickness regime, the tunnel magnetorezistance effects are investigated both in static and dynamic (low frequency) regime. We discuss the possibility to tune the transport characteristics by interfacial chemical and electronic structure engineering.

Plenary Pl-15

Beijing Synchrotron Radiation Facility and Its Application in Nanoscaled Materials

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Abstract. The present status of Beijing Synchrotron Radiation Facility (BSRF) is briefly introduced in this report. SR-based X-ray diffraction (XRD), small angle X-ray scattering (SAXS), and X-ray absorption fine structure (XAFS) techniques were used to probe the structural changes of nanoscaled materials. For example, the structural stabilities of germanium oxide nanomaterials with different surfactants were investigated. The interfacial change in Au@SiO_2 core-shell nanoparticles was detected. The thermal expansion behaviours of Ni and Co metal nanowire arrays were measured. The growth process of Pt and Au nanoparticles were monitored. All these studies demonstrate that SR-based X-ray experimental techniques can be well used to in-situ and real-time study on the structural changes of materials. A high-brilliance high-energy third-generation SR source is expected to be constructed in China.

Section T1:

Molecular, biomolecular and environmental systems

Oral T1-1

The investigation of pictural materials of a Transylvanian diptych wooden icon

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Abstract. In order to preserve a wooden icon belonging to the Transylvanian Ethnographic Museum collection the scientific expertise of the wooden support and of the pictural materials (ground, pigments, binder and varnish) used for the „*Virgin Mary with the Child*” and „*Diptych*” diptych icons (8228 inventory number) were investigated by FTIR spectroscopy, EI-MS spectrometry and DSC thermal analysis. FTIR spectroscopy and DSC methods offer information about the wooden support whereas EI-MS and FTIR methods were employed for binder, varnish and pigments structural characterization. These structural data can be correlated with the artistic, theological and historical analysis of this religious patrimony object.

Oral T1-2

Chitosan-based carriers with anti malaria's

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Abstract. The objective of this research was to synthesize and characterize chitosan-based liquid and solid materials with unique absorptive and mechanical as carriers for quinine – one of the most used anti malaria's drug. The use of chitosan (CTS) as base in polyelectrolyte complex systems, to prepare solid release systems as sponges is presented. The preparation by double emulsification of CTS hydrogels carrying quinine as anti-malaria's drug is reported. The concentration of quinine in the CTS hydrogel was 0.08 mmol. Chitosan – drug loaded hydrogel was used to generate solid sponges by freeze-drying at - 610°C and 0,09 atm. Structural investigations of the solid formulations were done by Fourier-transformed infrared spectroscopy (FTIR), ultraviolet-visible spectroscopy (UV-VIS), spectrofluorimetry, differential scanning calorimetry (DSC) and X-ray diffractometry. The results indicated that the drug molecule is forming temporary chelates in CTS hydrogels and sponges. Electron paramagnetic resonance (EPR) demonstrates the presence of free radicals in a wide range and the antioxidant activity for chitosan – drug supramolecular cross-linked assemblies.

Oral T1-3

Determination of anionic surfactants in water samples using GC/MS system

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Abstract. Linear alkylbenzene sulfonates (LASs) are the most commonly used anionic surfactants in diverse industrial, household and commercial applications. The extensive use of LASs in the formulation of domestic and industrial detergents results in thousands of tons of this contaminant being incorporated into wastewaters. Given this situation, numerous studies have been undertaken directed towards the degradation of LAS in wastewater treatment plants, since degradation is the only process able to eliminate LAS.

These surfactants have a strong affinity for sorption to sediments. However, data regarding the fate and effects in sediments following release into the environment have not been reported in great detail. The studies concluded that degree of degradation is depending of individual structure of LAS. Therefore for detailed studies of degradation and sorption, analytical methods for determination of every compound from LASs family are crucial.

This work presents:

I) A simple and rapid method to analyse alkylbenzenesulfonates (LASs) in water samples using GC-MS system after SPE extraction;

II) A study of the Electron Impact mass spectra of individual isomer of LASs.

Oral T1-4

Ionic co-crystals of calcium chloride: possible applications in the Pharmaceutical Industry

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Abstract. The use of electrostatic interactions such as those present in ionic co-crystals containing alkali metals and alkaline earth metals compounds has never been systematically explored in the field of Crystal Engineering. In these structures the interaction between inorganic ions and organic molecules must be seen as a special case of solvation, with the organic molecules acting as a solvent molecules (in competition with water if present) for ions.1 In primary and secondary amides, N-H and C=O dipoles act respectively as donor and acceptor for hydrogen bonds, thus with the possibility of solvating inorganic salts. We investigated the “solvation properties” of a number of molecules some of which are active pharmaceutical ingredients (APIs): barbituric acid, diacetamide, malonamide, oxamide, urea, nicotinamide and piracetam. As for the inorganic counterpart, $CaCl_2$ salt was chosen because of its non-toxicity and potential applications in the Pharmaceutical field. Synthetic methods varied from classical crystallization from solution, to slurry, mechanochemical solid state techniques (grinding and kneading), and solid-gas techniques (vapor-digestion). Crystal structures were solved either from single crystal data, or by powder diffraction using simulated annealing procedures. All crystalline compounds were analyzed with DSC, TGA and variable temperature XRD. Dissolution rate measurements were performed on ICCs of APIs.

Oral T1-5

Thermodynamics of bioligands binding to nanogels investigated by nanocalorimetric techniques

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Abstract. Nanohydrogels are polymeric nanoparticles made from porous hydrophilic polymers structured as a cross linked macromolecular network. By optimizing the polymer network structure, the binding efficiency may be improved. The nanohydrogels offer many advantages as polymer-based molecular binding systems: i) a tunable size from tens of nanometers to micrometers, ii) a large surface area appropriate for multivalent bioconjugation, iii) a functionalized internal network for the incorporation of small bioligands and iv) the possibility to attach electric charges on the nanoparticle surface and to control the charge density.

Polymeric nanoparticles based on poly(N-isopropylacrylamide) (PNIPA) and poly(acrylic acid) (PAA) have been characterized by Isothermal Titration Calorimetry (ITC) technique. These materials have been increasingly exploited as efficient binding systems and are intensively used as delivery vectors.

The types and the number of binding sites N per nanoparticle as well as the corresponding binding constant K, and the reaction enthalpy ΔH have been obtained for several biomolecules. If the small molecules are attached by noncovalent intermolecular interactions and can penetrate inside the polymeric particle, the large biomolecules like proteins bind at the nanoparticle surface, mainly by electrostatic forces.

Poster T1-1

Determination of colorant compounds from food by Gas Chromatography/Mass Spectrometry methods

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Abstract. Flavonoids and carotenoids are main classes of natural colorants, being responsible for the colour of a wide variety of foodstuffs and beverages. In the last years, the interest for analyzing of these colorants in food and drinks increased, specially to determine their antioxidant activity and, in the case of juices, to check them for possible adulterants. A simple and rapid method using GC/MS system was developed for determination of natural colorants present in different beverage. Prior to GC/MS analysis, the samples were subjected to concentration and than to a hydrolysis/methylation process using as reactants the organic base tetramethylammonium hydroxide (TMAH). Detection was performed in full scan mode and compounds were identified based on mass spectra.

In every sample were identified fragment molecules as result of thermal decomposition of original compounds. The fragment compounds can be used as valuable markers for flavonoids or carotenoids and is shown by selected ions chromatogram profiles. Theirs relative abundance is used as indicator for sample origin.

Poster T1-2

Solvent effect on the anharmonic vibrational frequencies in Guanine - Cytosine base pair

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Abstract. We present an *ab initio* study of the vibrational properties of cytosine and guanine in the Watson–Crick and Hoogsteen base pair configurations. The results are obtained by considering the DFT method together with the Polarizable Continuum Model (PCM) using PBE and B3PW91 exchange-correlation functionals and triple ζ valence basis set. We investigate the importance of anharmonic corrections for the vibrational modes taking into account the solvent effect of the water environment. In particular, the unusual anharmonic effect of the H^+ vibration in the case of the Hoogsteen base pair configuration is discussed.

Poster T1-3

^{1}H NMR study of the inclusion complex between β – CD and flurbiprofen

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Abstract. The complexation between flurbiprofen and β – CD was investigated in solution by 1D and 2D proton NMR. The induced chemical shifts variation in 1D NMR spectra were used to construct the Job plots and to calculate the association constant, K. The presence of R- and S-isomers of flurbiprofen is put in evidence in some 1D NMR spectra of β-CD / flurbiprofen. The geometry of the inclusion complex is analysed based on 2D NMR data.

Poster T1-4

Structural investigation of ambazone with lactic acid

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Abstract. Much research has been carried out on the preparation of pharmaceutical solid forms in order to improve their physical-chemical parameters such as solubility, dissolution rate of the drug, chemical stability and hygroscopic parameter. This study was dedicated to characterize the structural properties of the ambazone (AMB) with lactic acid (LA) solid form. The modality of obtaining new forms occurred starting from the ambazone with lactic acid (1:1), by grinding method at constant temperature. The obtained compound was investigated by X-ray powder diffraction (PXRD), thermal analysis (DSC, TG-DTA) and infrared (FTIR) spectroscopy. The difference between the PXRD patterns of AMB-LA and of the starting compounds evidenced a new compound. Using X-ray powder diffraction method, the lattice parameters were determined. Thermal and FTIR measurements on the pure compounds and on the (1:1) grinding mixture of AMB with LA confirm the new salt form formation.

Poster T1-5

Photopyroelectric measurement of thermal effusivity of volatile liquids. Thermal wave resonator cavity method.

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Abstract. The front photopyroelectric (FPPE) configuration, together with the thermal-wave resonator cavity (TWRC) method was applied in order to measure the thermal effusivity of volatile liquids. The methodology is based on a 4-layer detection cell (pyroelectric sensor, coupling fluid, solid separator and backing) in which the volatile liquid accommodates a special designed cell, in backing position. The value of the thermal effusivity of the volatile liquid sample is obtained as a result of a scan of the phase of the FPPE signal as a function of coupling fluid's thickness (TWRC method). The suitability of the method was demonstrated with investigations on several liquids as ethanol, acetone, hexane, ether, ethyl acetate. This alternative method is recommended when the classical frequency and/or thickness scanning procedures cannot be performed directly on the investigated liquid, due to its volatility.

Poster T1-6

Self-consistent measurement of all thermal parameters of a liquid by FPPE-TWRC technique

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Abstract. The front photopyroelectric (FPPE) configuration, together with the thermal-wave resonator cavity (TWRC) method was applied in order to measure both thermal effusivity and diffusivity of liquids. The methodology is based on a 4-layer detection cell (pyroelectric sensor, coupling fluid, solid separator and liquid backing) in which the investigated liquid is inserted successively in backing and in coupling fluid's position, respectively. When inserted in the backing position a scan of the phase of the FPPE signal as a function of (a known) coupling fluid's thickness (TWRC method) leads to the direct measurement of liquid's thermal effusivity. Inserting then the investigated liquid in coupling fluid's position (with a known backing liquid), a similar thickness scan leads to the measurement of its thermal diffusivity. In such a way the FPPE-TWRC method becomes self-consistent; all static and dynamic thermal parameters can be derived with the same technique (two of them are directly measured and the remaining two calculated). The suitability of the method was demonstrated with investigations on several liquids as water, ethylene glycol, glycerine, various oils.

Poster T1-7

Application of cyclodextrins in different routes of pharmaceutical forms administration

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Abstract. In this article the use of cyclodextrin in the different routes of drug administration it is explained. The review article gives the chemistry of cyclodextrins and addresses the issue of the mechanism of drug release from cyclodextrin complexes. Dilution, competitive displacement, protein binding, change in ionic strength and temperature and drug uptake by tissues are the different release mechanisms of the drug from the drug-cyclodextrin complex discussed here. The use and its limitations in the different drug delivery systems like nasal, ophthalmic, transdermal and rectal drug delivery are explained.

Poster T1-8

Analysis of the crystal packing patterns in Ethoxzolamide by SS-NMR

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Abstract. Solid State Nuclear Magnetic Resonance (SS-NMR) and molecular modelling in extended periodic systems are used to validate crystal structure of Ethoxzolamide (6-ethoxy-1,3-benzothiazole-2-sulfonamide) determined by X-Ray powder diffraction (XRPD). Using NMR CASTEP module of Materials Studio software package the results of quantum chemical computions of ^{13}C and ^{15}N chemical shieldings are compared with the measured chemical shifts, and important insights into the crystal packing patterns are obtained.

Poster T1-9

The Photochromic 2-(2',4'-dinitrobenzyl)pyridine. Electronic structure calculations.

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Abstract. The mechanism of the photoinduced nitro-assisted proton transfer (PNAPT) responsible for the photoactivity of 2-(2′,4′-dinitrobenzyl)pyridine (a-DNBP) is studied using (time-dependent) density functional theory in ground and excited electronic states.

The recently developed M06 hybrid functionals of Truhlar and Zhao with basis sets up to Dunning’s correlation consistent triple-zeta, aug-cc-pVTZ, are used to calculate the minimum energy conformers and the transition states between the three closed-shell tautomers of a-DNBP. This system, due to the very small structural change experienced by the surrounding during PNAPT, is promising for the design of photoactive systems maintaining their crystallinity during a prolonged operation.

Poster T1-10

DFT study of cysteine adsorbtion on gold defect surfaces

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Abstract. The controlled self-assembly of functional molecular species on well defined surfaces is a promising approach toward the design of nanoscale architectures. By using this methodology, regular low-dimensional systems such as supramolecular clusters, chains, or nanoporous arrays can be fabricated. Small biological molecules such as amino acids represent an important class of building blocks that are of interest for molecular architectonic on surfaces because they inherently qualify for molecular recognition and self-assembly. The interaction between amino acids and solid surfaces is decisive for the development of bioanalytical devices or biocompatible materials as well as for a fundamental understanding of protein-surface bonding. Their practical implementation often involves surface structural defects. We investigate the adsorbtion mechanism of the cysteine on Au(111) defect surfaces by means of the DFT. Our main concern is to describe the molecule-metal bonding mechanism. Therefore we present a complex study, including the full determination of the density of states for the free and adsorbed molecule, the determination of molecule-surface bonding energy. The method of crystal orbital overlap populations is used in order to determine the contribution of specific atomic orbitals to the molecule-metal bond.

Poster T1-11

Molecular Spin Change and Adsorbate-Substrate Decoupling by Ligand Attachment to Iron Phthalocyanine Molecules

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Abstract. By using x-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) we have investigated the interaction of iron phthalocyanine (FePc) adsorbed on a Au(111) surface with different electron donor and electron acceptor small molecules which function as ligands. The results show that ligand adsorption significantly affects the electronic structure at the interface through the formation of iron-ligand bonds. The formation of the iron-ligand bond decouples the FePc molecules from the Au(111) substrate, leading to a reorganisation of the Fe 3*d* states. The electronic structure changes lead to changes in the spin state of the iron atom; both a lowering of the spin state or complete spin quench are observed, depending on the ligand. Our findings show that the FePc-substrate interaction and molecular spin on the iron atom can be tuned by adsorption of molecular ligands. The results are in line with previous studies, which have studied the possibility of inducing changes into the electronic structure of surface adsorbates by ligand attachment or by atom-by-atom manipulation, indicate that a precise tuning of the bond strength and spin state of the FePc molecules by ligand attachment is within reach.

Poster T1-12

Determination of optical constants of polymethyl methacrilat films from IR reflexion-absorption spectra

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Abstract. The transmittance values measured in IR reflection-absorption (RA) spectra were used to determine the optical constants of dielectric films laid on solid substrates. To obtain the optical constants of polymethyl methacrilate films laid on steel we used dispersion analysis. In this case, the optical constants are obtained from IR spectrum recorded at a single incidence angle. The use of dispersion analysis offers the advantage of processing a large volume of data. This method is more flexible than the Kramers-Kronig analysis and can be applied to more complicated geometry of the spectrum. The shifts of absorption bands in reflectance-absorption spectra towards higher frequencies compared with absorption bands in transmission spectra were observed. Such effects are of importance, for example, in understanding the chemical and structural nature of thin films by interpretation of spectral shifts relative to bulk transmission bands.

Poster T1-13

Structural characterization of ambazone salt with nicotinic acid

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Abstract. Salt formation is a good method of increasing solubility, dissolution rate and consequently the bioavailability of poor soluble acidic or basic drugs. The aim of this study was to obtain and to investigate the structural properties of the compound that was obtained by solvent drop grinding method at room temperature starting from the 1:1 molar ratios of ambazone (AMB) and nicotinic acid (NA). The obtained compound was investigated by thermal analysis (DSC, TG-DTA), X-ray powder diffraction (PXRD) and infrared spectroscopy (FTIR). The difference between the patterns of AMB-NA and of the starting compounds evidenced the formation of a salt. Using X-ray powder diffraction data, the lattice parameters were determined. The thermal and FTIR measurements on the pure compounds and on the (1:1) grinding mixture of AMB with NA confirm the salt formation.

Poster T1-14

Change the antioxidant character of basil by growth in microwave field

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Abstract. An antioxidant is a molecule capable of inhibiting the oxidation of other molecules. As oxidative stress appears to be an important part of many human diseases, the use of antioxidants in pharmacology is intensively studied, particularly as treatments for stroke and neurodegenerative diseases. Natural antioxidants are used in medicine, preservatives in food and cosmetics and preventing the degradation of rubber and gasoline. In our work the antioxidants from reference and irradiated basil with microwave were determined. In this aim, the extracts were obtained by sonication in water:ethanol (40:60, v/v). These extracts were analysed by three methods: DPPH, ORAC and TROLOX. It was observed that the quantity of antioxidants increases in irradiated basil comparatively with reference basil.

Poster T1-15

The efficiency of different sampling methods for analysis of organic pollutants in surface waters

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Abstract. In our analysis, the sampling is generally performed by one of three methods: grab sampling, composite sampling or passive sampling. A grab sample is collected at a particular time and place representing only the composition of the source at that time and place. Composite sampling consists of a collection of numerous individual discrete samples taken at regular intervals over a period of time, usually 24 hours. The material being sampled is collected in a common container over the sampling period. Passive sampling can be defined in its broadest sense as any sampling technique based on free flow of analyte molecules from the sampled medium to a receiving phase in a sampling device, as a result of a difference between the chemical potentials of the analyte in the two media. In this study, we compared the results obtained by all this three sampling methods, for the detection of organic pollutants including herbicides, drugs, fragrances, plasticizers, and other components of industrial, domestic and agricultural origin in surface waters. The samples was collected from surafce water and analysis were performed by gas chromatigraphy/mass spectrometry system.

Poster T1-16

Synthesis and characterization of bentonite chemically modified with γ-aminopropyltrimethoxysilane

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Abstract. The bentonite, a colloidal native hydrated aluminium silicate clay consisting principally of montmorillonite (complex aluminosilicate, $Al_2O_3.SiO_2.H_2O$) has marked adsorptive properties A new polar stationary phase for thin-layer chromatography has been prepared by reaction of γ-aminopropyltrimethoxysilane with bentonite. The surface chemical modification were determined by elemental analysis, specific surface area measurement, FTIR spectroscopy, thermoanalysis and TLC.

Poster T1-17

Cyclodextrin-cardiovascular drug complexes investigated by nanocalorimetric methods

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Abstract. The aim of this work is to investigate the complexation of atenolol and captopril with various cyclodextrins (α-cyclodextrin, β-cyclodextrin and hydroxypropyl- β-cyclodextrin). The thermodynamics of complexation process is investigated by a very sensitive Isothermal Titration Calorimetry (ITC) technique. The results show that for both cardiovascular drugs the binding process has an exothermal nature. The entropic component ($T\Delta S$) for all binding processes is positive bringing a larger contribution to the negative change of Gibbs free energy (ΔG) than the enthalpy (ΔH). The positive entropic contribution is mainly established by two reasons. First is the insertion into the molecular hole of CD of the included part of the guest molecule that has a negative contribution to the entropy. The other is the release of water molecules from the cavity which bring the main positive contribution. The affinity of cyclodextrins for the atenolol is higher as compared to the affinity for captopril. Among the investigated cyclodextrins, atenolol has the highest affinity for β-cyclodextrin and captopril bind only the α-CD. The stochiometry of the binding processes ($n < 1$) suggest that supramolecular structure obtained by complexation is a sandwich-type architecture in which the drug molecule is squeezed between to CD molecules.

Poster T1-18

Surface-enhanced Raman spectroscopy and DFT calculations on benzylpenicillin

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Abstract. Benzylpenicillin, commonly known as penicillin G, is the gold standard type of penicillin, used to treat infections and inflammations and typically given by parenteral administration because it is unstable in the hydrochloric acid of the stomach. Benzylpenicillin serum concentrations can be monitored either by traditional microbiological assay or by more modern chromatographic techniques. However, these standard methods for benzypenicillin analysis are complex, laborious and require a dedicated laboratory environment. As a cost-effective and less time consuming alternative, surface-enhanced Raman scattering (SERS) spectroscopy in conjunction with quantum chemical calculations can be used for monitoring and identification of drugs in low-concentrated solutions. SERS spectra of benzylpenicillin have been assigned based on Density Functional Theory (DFT) calculations at B3LYP/6-31G(d) level of theory in order to characterize the structural and vibrational properties of this molecule. As SERS “marker bands”, useful to identify and monitor benzylpenicillin, we mention the band at 575 cm^{-1}, with the calculated correspondent value at 577 cm^{-1}, assigned to the bending vibration of the angle (C<C<C) ,defined by two CH_3 groups and the C atom between them. The most enhanced band in the SERS spectra, at 1000 cm^{-1}, is predicted by the calculation at 979 cm^{-1} and it is assigned to the ring “breathing” vibration.

Poster T1-19

The use of Mass Spectrometry in the artwork studies

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Abstract. In the last decade Mass Spectrometry (MS) becomes a very powerful tool for the identification of organic materials from artworks. Beside its great potential to resolve molecular structures, this technique does not require sample pre-treatments, thus avoiding risks in sample manipulations and is a time-saving technique. In opposition to other techniques MS coupled with Gas Chromatography (GC/MS) eliminates compounds interference. The layered structure of icon were revealed frequently using GC/MS system. The protective varnish (mixture of resin with draying oil) characteristics is used to identify the ages or author of artwork.

The paper shows icon characteristic obtained from measurement on diagnostic ions of varnish sample in a Mass Spectrometer with direct introduction inlet system (DI-MS).

Poster T1-20

Synthesis and structural studies of trianglimine macrocycles with triptycene and anthracene rotors

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Abstract. Macrocyclic compounds have found applications in many fields of chemistry, from binding cations, anions or neutral molecules to building molecular machines that can reproduce at molecular level some of our daily life tools. One type of macrocycles are Schiff base macroclyces formed in the reaction of dialdehydes with diamines. In the present work the Schiff base macrocycles were synthesized as a result of condensation reaction [3+3] between *1R,2R*-diaminocyclohexane and dialdehydes with triptycene and anthracene backbone. In order to evaluate the movement of the triptycene moieties, which can be considered as paddles inside the macromolecular structure we performed kinetic studies of the obtained macrocycle. The investigation was carried on by using dynamic ^{1}H NMR at different temperatures and by circular dichroism (CD), respectively. Molecular modelling studies were applied for the generation of theoretical rotamers of homologous structures derived from dialdehydes and cyclohexylamine for stereochemical studies.

Poster T1-21

Preparation and characterization of urea – oxalic acid solid form

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Abstract. The selective production of crystalline polymorphs is an outstanding problem in solid-state chemistry. In this study, the preparation of a new urea solid form is based on pure urea and oxalic acid (1:1), by grinding the components at room temperature. The resulted compound was investigated by X-ray powder diffraction (PXRD), thermal analysis (DSC, PPE) and infrared (FTIR) spectroscopy. The difference between the PXRD patterns of urea-oxalic acid and of the starting components evidenced a new compound. Using X-ray powder diffraction method, the lattice parameters were determined. Some thermal properties of the obtained compound were also investigated by the previous mentioned calorimetric techniques.

Poster T1-22

Analysis of (D/H) isotopic ratios of some Romanian wines by ^{2}H NMR

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Abstract. In the early 90`s the EU adopted the ^{2}H-NMR method for wine analysis as an official method (EEC 2676/90), in order to tackle the problem of over-chapitalization of wines in Europe. A deuterium natural abundance quantitative NMR method (SNIF-NMR: Site -specific Natural Isotope Fractionation) was developed as an efficient and powerful tool capable of characterizing the chemical origins of organic molecules and distinguishing their biological and geographical origin. The SNIF method is based on the measurement of deuterium / hydrogen (D/H) ratios at the specific sites of the ethanol. Using this method we present the obtained results for a series of Romanian wines.

Poster T1-23

Dosing V(V), Cu(II), Pb(II), Cd(II) in waters of the Prut River by the cathodic voltammetry

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Abstract. The work is focused towards applying methods developed throughout the study of the electrochemical behaviour of heavy metals (V, Cu, Cd, Pb) on the mercury electrode in the presence of a number of complexing agents. So, 2,3-dihydroxy-benzaldehyde (2,3-DHBA), thiosemicarbazide-diacetic acid (TSCDA), semicarbazone 8 - quinolinaldehyde (SCQA) and 4-phenylthiosemicarbazide (4-FTSC) have served as agents of accumulation for dosing V (V), Cu (II), Pb (II), Cd (II) by the adsorptive cathodic stripping voltammetry. The metal ions form with these reagents complexes that are adsorbed on the dropping and stationary mercury electrode.

The accumulation time of analyzed species on the suspended mercury drop is dictated by the interference of other species, is dependent on the metal nature and varies within 10 - 180 s. The accumulation potential has been optimized in function of the nature of the reagent and the metal. For a linear potential sweep (1 V / s), the function $I_p = f(C_M)$ is linear under conditions of stationary diffusion, mercury electrode with suspended drop, and allows to be determined the following minimum concentrations: $2 \cdot 10^{-10}$ M V(V) (2,3-DHBA-BrO_3^-, $t_{ac} = 30$ s), $5 \cdot 10^{-9}$ M Cu (TSCQA, $t_{ac} = 60$ s); $4 \cdot 10^{-9}$ M Cd (FTSC, $t_{ac} = 30$ s) and $2 \cdot 10^{-7}$ M Pb (SCQA, $t_{ac} = 10$ s). The two developed methods have been applied to the determination of these metals in the waters of the River Prut.

Poster T1-24

Forecasting the fate of heavy metals in contaminated ecosystems

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Abstract. Although chemical analytical measurements are necessary to investigate the composition and magnitude of sediment contamination and to identify possible contaminant sources, these determinations, alone, are inadequate tools for fully characterizing and predicting potential biological effects in contaminated aqueous ecosystems. Having only this information, it is impossible to predict the future development of the metal amounts and its species in contaminated ecosystems under the change of environmental conditions (e.g., pH, Eh, cations, organic matter and other metal-complexing ligands). For a risk assessment of contaminated sites, or for natural attenuation process management, it is of primary importance to know how and to what extent the contaminants will spread or fall in concentration in the future. Thus, the problem of controlling the ion concentrations in natural systems may be formulated as: what is the response of the system when changing the parameters that govern the pX (negative logarithm of ion activity)? Using our developed buffer approach may yield extended knowledge and a deeper understanding of the processes that control the concentrations of components as well as a powerful tool for the assessment and prediction of long-term effects in natural attenuation as a remediation alternative within contaminated environmental systems.

Poster T1-25

Solid forms of indapamide: structural studies

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Abstract. Indapamide (IDP) is a non-thiazide sulphonamide diuretic drug generally used for the treatment of essential hypertension. The aim of this work was to obtain and to characterize new solid forms of IDP. In this respect, the recrystallization of IDP from different solvent or solvent mixtures was carried out. Thermoanalytical techniques (differential scanning calorimetry (DSC) and thermogravimetry (TG)), X-ray powder diffraction (XRPD), Fourier transform infrared spectroscopy (FTIR), solid state nuclear magnetic resonance (NMR) spectroscopy and scanning electron microscopy (SEM) were used for structural characterization of the new obtained solid forms. Based on the results of these techniques we can conclude that IDP recrystallised from acetonitrile, acetonitrile+ dichloromethane and acetonitrile+ diethyl ether solvent mixtures present different structures and physical properties as compared with the starting IDP.

Poster T1-26

Determination of some volatile compounds in spirit drinks by headspace solid-phase microextraction gas chromatography – mass spectrometry

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Abstract. The volatile composition of some spirit drinks was studied by headspeace soild-phase microextraction (HS-SPME) method coupled with gas chromatography – mass spectrometry (GC-MS). Some volatile compounds, such as alcohols, ethyl esters, fatty acids and terpenes are mainly responsible for the flavour of alcoholic beverages and their amounts specify the quality of the spirit drink. From this perspective it is interesting to develop a rapid, selective and sensitive analytical method that enables the simultaneous quantification of the principal molecules identified as responsible for the organoleptic characteristic of alcoholic beverages. Several spirit drinks were analyzed in order to characterize the volatile profile and to make a comparison between the home made and commercially available alcoholic beverages. The results obtained from fruit and corn product are comparated and discussed. The SPME extraction was preferred due of the fact in this way was eliminated the use of solvent and therefore the interference with analytes.

Poster T1-27

Determination of flavonoids in *Triticum aestivum L.* treated with ampicillin

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Abstract. Pharmaceutical residues in the environment, and their potential toxic effects, have been recognized as one of the emerging research area in the environmental chemistry. Antibiotics can reach plants from treated soil or due to irrigation. The flavonoids extraction from *Triticum aestivum L.* treated with ampicillin and separation of flavonoids are presented in this study. There were used classical and modern extraction techniques (maceration, microwave assisted solvents, etc). The efficiency of extraction process was spectrophotometricaly evaluated by determining the total flavonoids content and by HPTLC on silica gel plates using the mixture: petroleum ether – acetone – formic acid (35:10:5, v/v) as mobile phase. The developed plates were inspected both in ultraviolet and visible after visualisation with NTS reagent (diphenylboryloxyethylamin). The chromatographic plates were compared in respect to determine the changes in extract composition due to the different extraction techniques. Depending on the concentration of ampicillin administered to plants, comparative studies on flavonoids content were performed.

Poster T1-28

Identification of flavonoids from parsley extracts by HPLC analysis

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Abstract. Flavonoids are phenolic compounds isolated from a wide variety of plants, and are valuable for their multiple properties, including antioxidant and antimicrobial activities. In this work, parsley (*Petroselinum crispum*) extracts were obtained by three different extraction techniques: maceration, sonication and microwave-assisted solvent extraction. The extractions were performed with ethanol-water mixtures in various ratios. From these extracts, flavonoids like the flavones apigenin and luteolin, and the flavonol quercetin, were identified using an HPLC Shimadzu apparatus equipped with PDA and MS detectors. The separation method involved a gradient step. The mobile phase consisted of two solvents: acetonitrile and water with 0.1 % formic acid. The separation was performed on a RP-C18 column.

Poster T1-29

Biomolecules-mediated reactivity of gold nanoparticles

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Abstract. This paper reports the results of an investigation of the reactivity and assembly of gold nanoparticles mediated by cysteine (Cys), a thiol-containing amino acid found in plasma, and its dimmer cystine (BCys), respectively. Metallic nanoparticles, particularly gold (AuNp), are synthesized by photochemical reduction of metallic salts, dispersed in a polymer matrix, under ambient conditions. The citrate-capped metallic nanoparticles decrease the barrier to the cysteine derivatives adsorption onto the nanoparticles surface and facilitate the zwitterion-type electrostatic interactions between amino acid groups of cysteine derivatives bound to the nanoparticles. The evolution of the adsorption of these biomolecules on gold nanoparticles for S-functionalization was investigated by TEM and optical spectroscopic methods. The aim of our work is to gain insight into the biomolecules-AuNp interaction and reactivity, which has potential application for the detection of thiol-containing amino acids.

Poster T1-30

Analysis of polarization transfer efficiency in 2D ^{13}C correlation solid-state NMR spectra of uniformly enriched L-alanine

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Abstract. Efficient polarization transfer between ^{13}C nuclei in uniformly labelled organic compounds is an essential requirement for both, solid-state NMR spectral assignment and structure elucidation. The polarization transfer can be enhanced by using recoupling pulse sequences, which reintroduce the dipolar ^{13}C-^{13}C interactions. An experimental analysis of *phase-alternated recoupling irradiation scheme* (PARIS) efficiency for different mixing times and pulse length is discussed. Two-dimensional correlation spectra for ^{13}C uniformly labelled L-alanine acquired at moderate spinning frequency are presented.

Poster T1-31

Analysis of flavor compounds by GC/MS after liquid-liquid extraction from fruit juices

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Abstract. In this work, we described a rapid method for analyzing of volatile profiles of several commercial fruit juices using GC/MS instrument after liquid-liquid extraction. Volatile flavor compounds have been identified based on mass spectrum obtained in EI mode. This method allows to analyses a wide range of flavor compounds (esters, aldehydes, alcohols, terpenoids) the procedure was rapid, simple and inexpensive. Moreover, by means of volatile compounds it could be possible to distinguish between juices of organic and conventional production and those with flavorings addition. More of 20 compounds were identified and quantified as relative chromatogram area taken on larges ion in mass spectrum.

Poster T1-32

ICP-MS determination of heavy and rare metals in soils and sediments from Transylvania Area

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Abstract. Soil is a component subsystem of terrestrial ecosystem, resulted after multitudinous physical, chemical and biological processes. Sediment is a major source with nutrients for aquatic organisms. Its analysis is important in the assessment of total ecosystem (in addition to water and soil quality evaluation) because it does reflect the system quality at long-term range. Several soil and sediment samples were collected from adjacent raw water reservoirs from Cluj and Salaj districts. These samples were passed through out digestion processes in order to be brought into a suitable solution for ICP-MS analysis. High numbers of metal compounds were detected in these samples, their overall range being between 0.0005 – 1000 mg/kg. Metals transport through soil and sediment depends of its amount, soil and sediment properties and several other environmental parameters. Increased average levels of metals as As, Pb, U and Cd in dry periods could be explained by the missing of dilution processes through rain or other meteorological event.

The paper presents the obtained results and discusses its relative to quality standards.

Section T2:

Advanced technologies, applied research

Oral T2-1

Application Green IT for physics data processing at INCDTIM

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Abstract. Green IT is the next generation technology used in all datacenter around the world. Its benefit is of economic and financial interest. The new technologies are energy efficient, reduce cost and avoid potential disruptions to the existing infrastructure. The most important problem appears at the cooling systems which are the most important in the functionality of a datacenter. Green IT used in Grid Network will benefit the environment and is the next phase in computer infrastructure that will fundamentally change the way we think about and use computing power. At the National Institute for Research and Development of Isotopic and Molecular Technologies Cluj-Napoca (INCDTIM) we have implement such kind of technology and its support helped us in processing multiple date in different domain, as well as assure brought the Institute on the major Grid domain site with the RO-14-ITIM Grid site. In this paper we present benefits which the new technology brought us and the result obtained in the last year after the implementation of the new green technology.

Oral T2-2

What became of Cold Fusion in 2011?

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Abstract. The long story of Cold Fusion has radically changed in 2011 when a variant of the Ni-H Low Energy Nuclear Reaction was accomplished at the industrial level; the conditions for an energy source i.e intensity, reproducibility and controllability, continuity (duration of many months), safety and upscalability being all fulfilled.

Being an Cold Fusion veteran, I want to speak about the essentials of this reality and its implications for the future.

Oral T2-3

H_2-SCR at low temperatures on noble metal supported catalysts

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Abstract. The selective catalytic reduction of NO using hydrogen as reducing agent (H_2-SCR) is investigated on alumina supported noble metal catalysts at low temperatures (<300°C). Three noble metal supported catalysts (Pt/Al_2O_3, Pd/Al_2O_3, and Rh/Al_2O_3) were prepared by the incipient wetness impregnation method in order to obtain a metal loading of 1 wt.% on alumina. Characterization of catalysts was performed by N_2 adsorption-desorption at -196°C, XRD, NO temperature programmed desorption, and H_2 temperature programmed desorption. Catalytic activity tests of the investigated noble metal catalysts were performed under plug flow conditions, using a feed stream of 0.5% NO, 0.65% H_2 and Ar as balance gas, at temperatures below 300°C, at a GHSV of 4500 h^{-1}. Total NO conversion and high N_2 selectivity (>75%) were obtained for each catalyst, under different temperature conditions. The influence of the metal and of the reaction temperature is investigated towards the catalytic performance of the studied catalysts.

Oral T2-4

Basic Applications of Metal Hydride Technologies

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Abstract: Metal hydrides (MH) are promising materials for hydrogen based applications such as storage, purification and separation, thermal compression of hydrogen and a variety of energy conversion systems such as heat pumps and refrigerators. These applications require a thorough knowledge of important thermo physical and sorption properties of selected hydrogen absorbing alloys. In this paper we report our recent researches to develop: (i) an advanced stationary hydrogen storage system using, (ii) a metal hydride based water pump powered solar energy and (iii) a multi-stage hydrogen thermal compressor with 30:1 overall compression ratio. During the development of these applications, the studies were focused on the improvement of MH performances, acquired by tailoring of their properties and new technical solutions for hydrogen fast mass and heat transfer storage reactors. Some results obtained during testing of the prototypes are presented following up the operating parameters: supply pressure, storage volumes, cold and hot fluid temperatures, cycle duration. To improve the efficiency and economics of the hydrogen storage/compression process, all the developed systems can operate in conjunction with advanced hydrogen production technologies from renewable resources.

Oral T2-5

Functioning of protective UV filters based on gold nanoparticles

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Abstract. The aim of this work is to obtain and to simulate the functionality of the UV filters based on GNP. The filters, photochemically obtained, are based on GNP of various dimensions embedded in polymer matrix. The filters exhibit absorption maxima ranging from 527 nm to 600 nm and block the transmission of the radiation in near UV. In order to simulate the functionality of these filters, we use a spectral image processing algorithm. The algorithm allows us to perceive the effects of the filters on the text image.

Oral T2-6

Simultaneous determination of some artificial sweeteners in ternary formulations by FT-IR and EI-MS

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Abstract. Artificial sweeteners are widely used in food, beverage and pharmaceutical industries all over the world. In this study some non-nutritive sweeteners such as aspartame (AS), acesulfame–K (ACK), sodium cyclamate (SCY) and sodium saccharin (SSA) were simultaneously determined in ternary mixtures using FT-IR (KBr pellet technique) and EI-MS measurements. FT-IR method is based on direct measurements of the peak height values and area centred on 1737 cm^{-1}, 836 cm^{-1}, 2854 cm^{-1} and 1050 cm^{-1} for aspartame, acesulfame–K, sodium cyclamate and sodium saccharin, respectively. Mass spectrometry determinations show the characteristic peaks at *m/z* 91 and 262 for aspartame, *m/z* 43 and 163 acesulfame-K, *m/z* 83 and 97 for sodium cyclamate and *m/z* 104 and 183 for sodium saccharin. The results obtained by EI-MS in different formulations are in agreement with the FT-IR ones and provide also essential data concerning the purity grade of the components. It is concluded that FT-IR and EI-MS procedures developed in this work represent a fast, sensitive and low cost alternative in the quality control of such sweeteners in different ternary formulations.

Poster T2-1

DFT study of molecular monolayers on Si for memory applications

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Abstract. Within the current efforts made worldwide for miniaturization of electronic components, the search for new flash memories based on molecular architecture represents a major challenge. The focus of this research is on integrating redox-active molecules into Si structures, in order to develop a new class of hybrid silicon/molecular devices for memory applications. A physical and electrical investigation is proposed, where redox - active molecules act as storage medium. The various relevant electronic properties like HOMO LUMO gaps, partial atomic charges, density of states, relative energies of redox states, the influence of the charge transfer of molecular structures on their properties, the particular interaction between the molecule and substrate, are investigated in the framework of quantum chemistry DFT methods in combination with Solid State Physics theory. Our goal is thus to derive the optimum theoretical approaches based on DFT methods best adapted to the issues mentioned above, and to bring helpful interpretations of experimental findings based on the electronic structure.

Poster T2-2

Investigation of heat and mass transfer process in metal hydride hydrogen storage reactors, suitable for a solar powered water pump system

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Abstract: The paper analyzes heat and mass transfer process in metal hydride hydrogen storage systems as key element in the development of a solar powered pump system. Hydrogen storage and compression performance of the developed reactors are investigated according to the type of metal alloys, the metal hydride bed parameters and system operating conditions. To reach the desired goal, some metal hydride from groups AB_5 and AB_2 were synthesized and characterized using elements substitution for tailoring their properties: reversible hydrogen absorption capacity between the hydrogen absorption and desorption pressures at equilibrium at small temperature differences. For the designed hydrogen storage reactors, a new technical solution which combines the effective increase of the thermal conductivity of MH bed and good permeability to hydrogen gas circulation, was implemented and tested. The results permitted us to develop a heat engine with metal hydride, the main element of the functional model of a heat operated metal hydride based water pumping system using solar energy. This is a free energy system able to deliver water, at a convenience flow and pressure, in solitude places without conventional energy access.

Poster T2-3

Spectroscopic studies of copper ions doped in tellurate glasses obtained by sol-gel method

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Abstract. The preparation of copper nitrate doped tellurate glasses by sol-gel method and spectroscopic studies of this tellurate system are reported. FTIR spectroscopy results show that this glass consists of [TeO_6], [TeO_4] and [TeO_3] structural units and indicate that six-coordinated tellurium (VI) in [TeO_6] units were partially changed to four-coordinated tellurium (IV) in [TeO_4] units during the doping with $Cu(NO_3)_2$. EPR spectra of the studied glasses were obtained due to the presence of Cu^{2+} paramagnetic ions and reveal the local order in matrix, the distribution and valence state of cooper ions. Thus, the EPR spectra show a partially resolved parallel hyperfine structure and no resolved perpendicular structure. The EPR spectra could be a superposition of two signals, one due to isolated Cu^{2+} ions in axial neighborhood, and the other due to the presence of magnetically coupled Cu^{2+} species.

Poster T2-4

1,2,3-Triazolium ionic liquid tagged organocatalysts in organic synthesis

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Abstract. 1,2,3-Triazolium salts have been know for long. However, their potential as ionic liquids was recognized quite recently. The major trend in the use of triazolium ionic liquids involves tethering triazolium ionic liquids with catalytically active species such as (*S*)-proline. The resulting molecule can serve both as solvent and as catalyst. These catalysts are interesting not only due to their recyclability but also due to their outstanding tuneable properties. They can have wide liquid range, thermal stability, tuneable polarity, low flammability tuneable solubility and low vapour pressure along with ease of separation. The syntheses of 1,2,3- triazolium salts are mostly based on the so-called click reaction of organic azides with terminal alkynes. The *N*-alkylation of the resulting 1,2,3-triazoles can easily produce the 1,2,3-triazolium salts. This synthetic route has the advantage that there are four structural parameters, i. e. the alkyne, the azide, the alkylating agent and the counter anion in order to tune the properties of the resulting ionic liquid. Unlike the imidazolium ionic liquids 1,2,3-triazolium salts do not have acidic proton at position 2, which makes them appropriate for reactions under basic conditions. Consequently, they had been applied to aldol reactions, Michael additions and α-aminoxylation of cyclohexanone with nitrosobenzene.

Poster T2-5

Generating phase-matched high-order harmonics using CEP controlled few-cycle pulses

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Abstract. Recently was shown, by analytical calculations, that it is possible to freeze or to control the variation of the carrier-to-envelope phase (CEP) of propagated few-cycle laser pulses in the focal region. These methods consist in changing the variation of the beam's spot size for different spectral components at the focusing element and/or placing a dispersive slab (or medium) in the way of the propagating pulse. We developed a numerical method to calculate the electric field of the laser in these special configurations, which allowed us to simulate high-order harmonic generation (HHG) and perform phase-matching (PM) calculations for different types of CEP variations of the input pulse. HHG is assumed to take place in noble gas at low pressure and the interaction medium is placed close to the focal region of the pulse. During HHG and PM calculations we take into account the dispersion due to plasma contribution and neutrals. We assume that the electric field is perturbed during propagation and we perform PM calculations for different harmonic orders in the whole interaction region. We will present the effect of different CEP variations of the fundamental pulse on the high-harmonic spectra and explore the possibilities to obtain strong coherent HH radiation.

Poster T2-6

Acoustic Noise And Pneumatic Wave Vortices Energy Harvesting On Highways

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Abstract. This paper is aimed to present structure and principle of a energy harvesting sistem that uses the air movement emanated from passing traffic to produce and accumulate electrical energy. Each of the system's elements consists of a inertial mass panel which oscillate when driving cars pass. The panel is attached to a linear electromagnetic mini generator (or/and some piezo electric micro generators) and at the time of passing, it produces energy wich is store it in a supercapacitor or in a rechargeable battery. The concept can be applied to busy roads, and to high-frequented rail networks and it can work with street and road lighting, information panels and monitoring devices.

Poster T2-7

A miniaturized stirrer system for low viscosity fluids based on a rotating magnetic field generated by solenoids

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Abstract. Two methods of obtaining the spatially variable magnetic field for low viscosity liquid stirring have been implemented: one using a four pole electromagnetic system and one using a three pole magnetic system. The four pole electromagnetic system requires few electronic drive components and a simple driving algorithm, but it has the disadvantage of having a low packing arrangement. By contrast, the three pole electromagnetic system requires more electronic drive components and a more complex driving algorithm but this kind of structure has the most favourable packing arrangement of coils - possible for cylindrical shaped coil structures. The electromagnets' currents are controlled using a field – programmable – gate – array development board and a system of optical sensors. A magnetic piece, immersed in liquid, is spin by the rotating magnetic field. The stability of the spinning motion as a function of the driving command signal frequency has been studied for various liquid viscosities.

Poster T2-8

Magnetic clusters development in oxidized $CeNi_5$ powder

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Abstract. As advanced technologies are expanding, the need for novel functional materials significantly increases. Materials containing or consisting of nanosized metal particles have gained considerable attention in the last decades. Nanosized particles of ferromagnetic metals (Fe, Co, Ni) have been widely studied as they present an interest both for fundamental physics and potential applications such as catalysis, high density magnetic recording media, ferrofluids and medical diagnostics. Synthesis, X-Ray Diffraction (XRD), Transmission Electron Microscopy (TEM), X-Ray Photoelectron Spectroscopy (XPS), Raman spectroscopy and magnetic measurements at low temperature of Ni metallic clusters covered by NiO, Ce_2O_3 and CeO_2, obtained from $CeNi_5$ powder oxidized in air at different temperatures up to 800^oC, are reported. The average crystallite size of Ni core and the thickness of NiO oxide formed at the surface increase with temperature due to recrystallization processes, from 34 nm at 300^oC to 77 nm at 800^oC and from 9 nm to 19 nm, respectively. Ni metallic component was detected both in XPS valence bands and core levels spectra only after sputtering. The hysteresis loop presents a small shift towards negative magnetic fields which confirms the presence of ferromagnetic Ni/antiferromagnetic NiO interfaces.

Poster T2-9

Experimental measurements of the liquids dielectric properties changes with temperature in the 100MHz-20GHz range for microwaves power processing optimization

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Abstract. Relative permittivity and dielectric loss are the most significant dielectric parameters for the materials used in microwaves applications. These values are dependent of the material's temperature and the frequency of the microwaves field. In the microwaves power thermal processing it is important to know how the dielectric properties change with temperature, in order to better adapt the microwave generator with the reactor chamber. This paper presents the experimental measurements studies for dielectric properties of water in the temperature range of 1^0C to 90^0C. The measurements were performed with specific microwaves equipment, using the reflection method, in the 100 MHz - 20 GHz frequency range. Using measured permittivity values, the water probe impedance can be calculated for the entire temperature range. The mismatch adapting of the reactor (filled with the water probe) and the microwaves generator behaviour can be then evaluated.

Poster T2-10

Microwave generator for scientific and medical applications

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Abstract. Nowadays power microwave radiation is widely used in medical applications as hyperthermia, diathermy or ablation and for scientific applications such plasma generation, digestion, or as a catalyst in green chemistry. Nevertheless, designing a suitably adapted microwave generator that meets both the scientific and the more restrictive medical criteria remains a difficult task. We present here a simplified approach in designing such a microwave generator, according to the IEC60601 medical standard. The generator, based on a continuous wave (CW) magnetron, is coupled via a TE10 waveguide to feed either a hyperthermia applicator or a reactor chamber. Microwave interactions with the probe (or the tissue) depend strongly on the magnetron's power supply parameters and the impedance match of the entire microwave circuit. Any unmatched elements (magnetron to waveguide, waveguide to applicator, applicator to patient) give rise to a large voltage standing wave ratio (VSWR) which loads the generator with a surplus energy, converted to heat. Extra heating of the magnetron will deteriorate the amplitude of the generated microwave power field. We show here that, by using a proprietary patented temperature sensor sheet, we were able to detect and improve the impedance matching of the microwave circuit.

Poster T2-11

Single attosecond pulse generation by two laser fields

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Abstract. In this paper, the high order harmonic generation resulting from the superposition of two incommensurable frequencies is analyzed with the aim to find out the conditions that the relative intensity and frequency of the two fields have to fulfil in order to generate isolated attosecond pulses. It is observed that the two fields can be superimposed in both parallel and perpendicular polarization, both giving rise to a single attosecond pulse under appropriate conditions. The two geometrical configurations lead to similar output, and we anticipate the possibility to generate attosecond pulses shorter than 280 as and with energy centered around 80–100 eV.

Poster T2-12

High frequency atmospheric cold plasma treatment system for materials surface processing

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Abstract. The paper presents a new laboratory-made plasma treatment system. The power source which generates the plasma is based on a modern half-bridge type inverter circuit working at a frequency of 4 MHz, and giving an output power of about 200W. The inverter is fed directly from the mains voltage and features high speed protection circuits for both over voltage and over current protection, making the system light and easy to operate. The output of the inverter is connected to the resonant circuit formed by a Tesla coil and the dielectric barrier discharge plasma chamber. The plasma is generated at atmospheric pressure in argon, helium or mixtures of helium and small quantities of argon. It is a cold discharge ($T_{gas} < 150\ ^{o}C$) with a homogeneous structure. The plasma generates chemically active species, especially O and OH, which could be important in various applications such as the treatment and processing of materials surfaces.

Poster T2-13

The use of inductively coupled plasma mass spectrometry (ICP-MS) for the determination of toxic and essential elements in different types of food samples

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Abstract. Food is the primary source of essential elements for humans and it is an important source of exposure to toxic elements. In this context, levels of essential and toxic elements must be determined routinely in consumed food products. The aim of this study was to develop a suitable method for major and trace elements determination (essential and toxic elements) in different types of food samples (like rice, egg, meat, fish, bread, sugar, cheese, milk, butter, wheat, coffee, chocolate, biscuits pasta, etc.) by using inductively coupled plasma mass spectrometry (ICP-MS). Sample digestion is a critical step in most analytical methods for routine determination of chemical elements in food samples. In this study the Perkin Elmer Elan DRC(e) ICP-MS instrument was used; it provides an analytical method allowing a rapid, simultaneous determination of the concentration of nearly all the elements in the Periodic Table. Thirty metals were identified with concentrations obtained under the limits allowed for food samples.

Section T3:

Nanostructured materials and nanocomposites

Oral T3-1

An XAS study on Co – plasma polymerized HMDSN and Co_3O_4-SiO_x nanocomposites

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Abstract. Nanocomposites prepared with transition metals and their oxides embedded in an insulating polymer matrix have received much attention recently due to their new functional properties in optical, magnetic, and chemical applications. Cobalt – plasma polymerized hexamethyldisilazane (HMDSN) nanocomposites by RF magnetron sputtering of cobalt (PVD) and simultaneous plasma polymerization of the organo silicon monomer hexamethyldisilazane (PECVD) were successfully prepared. Also, we have prepared composites consisting of nanosized spinel type cobalt oxide particles embedded in an amorphous silicon oxide matrix (Co_3O_4-SiO_x composite). Co_3O_4-SiO_x composites have been prepared by calcination of initially prepared cobalt-plasma polymerized HMDSN nanocomposites. The electronic and the local structure were investigated using X-ray absorption near edge structure and extended X-ray absorption fine structure techniques.

Oral T3-2

Preparation and characterization of magnetic nanogels with temperature responsive core and pH responsive shell

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Abstract. We prepared water stable colloidal solution of magnetic microgels based on temperature-responsive N-isopropyl acryl amide (PNIPAm), pH responsive acrylic acid (PAAc) and nano size iron oxide ferrofluids (Fe_3O_4), in order to obtain dual sensitive magnetic materials with biological application. The FTIR spectra of P(NIPA-AAc) ferrogel samples, showed the absorption region of the specific chemical groups associated with PNIPA, PAAc and the Fe_3O_4 magnetic nanoparticles The morphology and the structure of the as prepared materials were confirmed by transmission electron microscopy (TEM) and the size distribution was determined by dynamic light scattering (DLS). Drug release experiments were performed using different type of biomolecules, like proteins or drugs, in simulated gastric and intestinal media. The amount of released compounds was determined by UV spectroscopy at characteristic wavelength of the biomolecules. In vitro drug release study showed that magnetic microgels displayed thermo and pH double responsive release behaviour.

Oral T3-3

The role of the reaction conditions on the morphological properties of few-layer graphene structures synthesized by radio frequency chemical vapor deposition

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Abstract. Few layer nano-graphene structures were successfully synthesized over various bimetallic MgO-supported catalytic systems. The reaction conditions such as synthesis temperature, flow rate and type of hydrocarbon, metal ratio in the catalytic system were varied and their effects on the morphological properties of carbon nano-structures were thoroughly studied. The bimetallic catalyst systems containing a combination of Fe/Co or Fe/Mo nanoparticles were employed to synthesize few to multi layer graphene sheets with a high crystallinity. It was found that as the flow rate of the hydrocarbon increased, so did the layer number and the diameter of the graphene structures synthesized utilizing a Radio-Frequency catalytic Chemical Vapor Deposition. Developing a proficient and low-cost method to produce high crystallinity and few-layer graphene sheets at a large scale is very important for many practical applications.

Oral T3-4

Hydrogen adsorption measurements on small amounts of samples

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Abstract. Hydrogen adsorption capacity of porous metal-organic frameworks (MOF) established this class of materials as one of the most promising hydrogen storage materials for on-board applications and fuel cell vehicles. The increasing number of papers focused on hydrogen uptake measurements on porous carbon materials and MOFs strongly require accurate data confirmed by measurements in different laboratories. As concerning the reliability of the literature data, it should be noted that measurements of H_2 adsorption isotherms needs special care, especially on small amounts of sample. A Round Robin exercise involving measurements in fourteen laboratories of pressure–composition–isotherms within the European project NESSHY. The results revealed remarkable scatter among participating laboratories, emphasizing the need to review methods, internal calibration or operability of analytical equipment and pointed out laboratories that might need a corrective action. The equipment of the volumetric Sievert type employed, sample cells and valves built-up in our institute are described. The cautions required in the various steps of the experiment in order to obtain accurate results are reviewed, including the equation of state for hydrogen gas for measurements down to 77K. Our measurements of hydrogen uptake on carbon nanofibers, Pt/activated carbon, MOF-5, MIL-101 and other materials are reported and compared to the available literature data.

Oral T3-5

Vibrational properties of DNA nucleotides adsorbed on Au(100) surfaces

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Abstract. The physical and chemical properties of molecules at surfaces play an important role in various fields, ranging from heterogeneous catalysis to nanoscale mechanics and organic optoelectronics. While the properties of individual molecules can be modified in a controlled manner by chemical synthesis, their anchoring at surfaces can give rise to new functionalities which may be used to design surfaces with specific properties. In order to reach such goals, a detailed characterization of the adsorption geometry is mandatory. One of the main tools developed in this direction is the vibrational spectroscopy. The SERS technique is one of the most efficient to be used in the characterization of molecular adsorption. Nevertheless, the interpretation of the vibrational spectra of the adsorbed molecules needs a careful analysis. We present here a theoretical approach, based on ab initio calculation. We apply the methodology to describe the vibrational properties of the nucleotides on gold surfaces. A comparison between the vibrational properties of the free and adsorbed nucleotides is also presented in order to get a better understanding of the adsorption mechanism.

Oral T3-6

Surface modification of magnetic nanoparticles by acrylates derivatives

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Abstract. Magnetic nanoparticles (NP) as magnetite (Fe_3O_4) have attracted researchers in various fields such as physics, medicine, and biology due to their multifunctional properties such as small size, superparamagnetism and low toxicity. Magnetic NPs are used for many applications such as drug delivery, cell separation, hyperthermia, diagnosis, sealing, waste water treatment, loud speakers and catalysis. To extend the application of magnetite NPs but also for hampering undesired aggregation, the surface of the Fe_3O_4 nanoparticles was widely modified with various biocompatible and biodegradable polymers. We report the synthesis and characterization of functionalized magnetite nanoparticles by polymer acrylate derivative. The polymerization of the acrylates derivatives takes place in the presence of stabilized magnetic NPs with unsaturated acids. The polymerization mechanism is a free radical polymerization initiated on the magnetic nanoparticle. The chemical structure of the obtained magnetic core-shell nanoparticles based on polyacrylates was determined by FT-IR and XPS spectroscopy. The morphology, structure and magnetic properties of the hybrid nanostructures were investigated by TEM and HRTEM, XRD spectroscopy and magnetization measurements. The cores are selected to possess superparamagnetic behaviour, while the polymeric shell serves as a protective layer, which can be functionalized lateron.

Oral T3-7

Magnetization enhancement of magnetic nanoparticles coated with polypyrrole

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Abstract. We are presenting the synthesis and characterization of hybrid structures obtained by coating “soft” magnetic nanoparticles like Fe_3O_4 and perovskite manganites of La0.67St0.33MnO3 (LSMO) type with polypyrrole (PPy). The thin amorphous layer of PPy was observed by HRTEM and analyzed by XPS and XANES techniques. The existence of superparamagnetism is evidenced by the very small values of coercive fields and FC and ZFC behaviors. The surface modification of the magnetic nanoparticles generates an increase of the saturation magnetization. This novel effect is attributed to a charge transfer process between the conducting polymer and the surface layers of the magnetic cores. As a result, a significant increase of the surface contribution to the overall magnetic moment of the nanoparticles is produced. The effect is correlated with the temperature dependences of coercive field and of the ESR integral intensities.

Oral T3-8

Dual efficiency of nano-structured TiO_2 / zeolite systems in removal of copper (II) and lead (II) ions from aqueous solution under visible light

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Abstract. The present study is targeted on solar photocatalytic removal of copper (II) and lead (II) ions from aqueous solutions using solar energy irradiated nano-structured TiO_2 / zeolite system. Citric acid has been used as hole scavenger. The influence of metal ions initial concentration and pH of the solutions on the removal process was investigated. The deposition value of the investigated metal ions, at pH 4, was higher with 46.3 % (for copper) and 41.8 % (for lead) when nano-structured TiO_2 / zeolite system was used in comparison with TiO_2 alone, thus being demonstrated the positive contribution of zeolite as adsorbent (due to its ion exchange capacity) to the photoactivity of TiO_2 nanoparticles. The percent of metal ions removal increase with initial concentration and in the range of pH 2 – 4. At pH values highers than 4 (between 4 and 7) a decrease of deposition percent for both investigated ions occurs.

Oral T3-9

Nanostructures based on metallic nanoparticles and biomolecules

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Abstract. Gold nanoparticles (AuNPs) have been intensively used for the surface modification of various systems due to their unique properties in the development of promising electrocatalytic or biosensing applications. We describe the preparation of a nanostructured assembly (amino acid layers/AuNPs) on the surface of a glassy carbon electrode (GCE). The results show that the amino acid layers/AuNPs can be used for the construction of composite materials with excellent electrocatalytic properties regarding the atenolol oxidation. The linear detection range for atenolol was varied and the lower detection limit was found to be of 3.9×10^{-7} M. Morphological and electrochemical characteristics of the nanostructured layer were investigated by Atomic Force Microscopy (AFM), Cyclic Voltammetry (CV), Linear Sweep Voltammetry (LSV) and Electrochemical Impedance Spectroscopy (EIS). In addition, we developed an equivalent electrical circuit to model the EIS data and to determine important parameters, such as the bulk resistance (R_b) of the PGA/cysteine/AuNPs assembly and charge-transfer resistance (R_{ct}). A similar approach (combination of amino-acids and metallic nanoparticles) can be further developed for the accurate and specific detection of various molecules.

Oral T3-10

Magnetically induced dichroism in concentrated magnetic colloids

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Abstract. We present and discuss experimental data that shows concave dependence on particle concentration of the reduced dichroism in magnetic colloids. The reduced dichroism is the dichroism divided by the particle concentration. With increasing particle concentration, the reduced dichroism peaks and above a certain concentration it monotonously decays. We discuss the experimental data in the frames of orientation, agglomeration and long-range interactions theoretical models for the magnetically induced dichroism in magnetic colloids. It was found that the concave dependence can be explained only by the long range interactions model developed by Socoliuc and Popescu (V. Socoliuc, L.B.Popescu, Physica A 390 (2011) 569) using the pair correlation function in magnetic colloids developed by Elfimova and Ivanov (E.A. Elfimova, A.O. Ivanov, Journ.Exp.Ther.Phys. 111 (2010) 146).

Oral T3-11

XPS and magnetic characterization of biocompatible polymers based magnetic nanostructures

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Abstract. Magnetic nanostructures designed either as core-shell nanoparticles or microgels may be obtained by simple procedures using water-based magnetic nanofluids and different polymers as starting materials. Magnetic core-shell type nanostructures were obtained by coating the magnetite nanoparticles of the magnetic fluid samples with pyrrole copolymer shells functionalized with different biomolecules such as glucose, biotin. Smart magnetic microgels were obtained by the copolymerisation of monomers N-isopropylacrilamide and acrylic acid or methacrylic acid in the presence of magnetic nanofluid. The magnetic nanostructures were investigated by TEM, DLS, XPS and magnetization measurements. Correlations between the synthesis parameters and particle magnetostatic properties, chemical surface composition, coating efficiency and embedding/encapsulation mechanisms of magnetic nanoparticles and particle clusters in polymers are discussed.

Oral T3-12

Influence of composition on the structure and macroscopic behavior of magnetizable fluids

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Abstract. The particle surface coating and volume fraction, as well as the size distribution and magnetic moment density of dispersed particles will be considered in correlation with carrier liquid properties, colloidal stability, magnetic and flow behavior of magnetizable fluids. Organic liquids and water carriers, magnetite and iron (nano) particles, saturated and unsaturated carboxylic acids and polymers were used to design magnetic fluids adapted to the requirements of applications, such as high pressure leakage-free rotating seals, semi-active vibration dampers or various biomedical uses. The structure, colloidal stability and macroscopic behavior of samples are discussed in terms of TEM, SANS, DLS, SLS, VSM and rotational rheometry measurements.

Oral T3-13

Progress of X-ray absorption spectroscopy techniques and nanomaterials application in Beijing synchrotron radaition facility

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Abstract. Understanding and tailoring structure of nanocrystals are of significant interest due to their potential structure-dependent properties. Here we focus on the x-ray absorption spectroscopy techniques and their application in nanomaterials. In Beijing synchrotron radiation facility, 1W1B-XAFS station is a general purpose instrument. Currently, the detection methods and sample environments are developed in XAFS station. 19 elements germanium array detectors system has been set-up and used for fluorescent XAFS of trace elements. It greatly extends the applications of XAFS in nanomaterials in life and environment science. On the other hand, mutifunctional in situ sample instruments has been improved, including liquid helium temperature in situ XAFS cell, liquid nitrogen temperature XAFS cell, liquid sample cell, high temperature and high pressure XAFS Instrument, which has supported XAFS measurements on the various conditions such as the low temperature, water solvent, organic solvent high temperature and also high pressure up to 40Gpa. Thanks to its versatility, it is useful to a broad scientific community, including ex-situ, along with in-situ study, which help to explore the electronic and local structure of nanomaterials. Furthermore understanding these structural properties of nanocrystals can trigger new opportunities and ultimately, new applications.

Poster T3-1

Highly porous MOF-template carbon for hydrogen storage

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Abstract. Development of highly porous materials is the main concern, in the last decades, for finding high hydrogen storage materials. Two classes of materials are of main importance: metal-organic frameworks (MOFs) and activated carbons (AC) with specific surface area over 2500 m^2/g. To obtain such high surface areas, for activated carbons, we used high surface area MOFs as template. $Cr_3O(OOC\text{-}C_6H_4\text{-}COO)_3$ (MIL-101) is a metal-organic framework synthesized by solvothermic method with a surface area of 3207 m^2/g. After impregnation of MIL-101 with furfuryl alcohol and polymerization at 80^oC, the MIL-101 template was removed by decomposition at 530^oC, at the same time with carbonization of the polyfurfuryl alcohol. The product is a mixture of templated carbon (TC) and Cr_2O_3 Two hydrogen adsorption measurements were done, on TC after removal of Cr_2O_3 and on $Pt/Cr_2O_3/TC$ by impregnation with Pt of the $TC\text{-}Cr_2O_3$ mixture.

Poster T3-2

The study of the photosensitive materials used in solar-hydrogen energy by a versatile photoelectrochemical cell

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Abstract. There were studied some photosensitive materials by using a versatile photoelectrochemical cell. The experimental arrangement makes possible the relative evaluation of the electrodes properties by measurement of the electric parameters, giving directly $I = f(U)$ for the cell electric circuit by using an “internal” chemical bias. It is also possible to measure the volume of the evolved gas, and to analyses it by a gas-chromatograph and by a mass spectrometer.

Poster T3-3

Few-layer graphene synthesized on the Au/MgO catalyst by CCVD-IH method

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Abstract. We present here the synthesis of few layer graphenes on a new catalytic system Au(1%)/MgO by Radio-Frequency Chemical Vapor Deposition, at 1000 ^{o}C, with methane as the carbon source (80 mL/min) and for various reaction times (30, 60 si 90 min). STEM analysis of the catalyst have indicated that the Au nanoparticles have dimenisons under 10 nm and are uniformly distributed over the MgO support surface. TGA measurements have shown that the synthesis yield increased with the reaction time and after a simple purification, (treatment with HCl 1:1) the purity varied between 98 and 98.4 %. Also it was found that the thermal decomposition of the graphenes increases with the synthesis time. TEM and Raman sample characterization post purification, have highlighted the presence of graphene layers with diameters in the orders of hundreds of nanometers and composed of 3-6 graphitic layers that are decorated with Au nanoparticles.

Poster T3-4

MOFs synthesis by microwave activation

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Abstract. Several MOFs were efficiently and quickly synthesized by a new method: microwave-assisted synthesis under atmospheric pressure. Their physicochemical and textural properties are similar or superior to those obtained by convective solvothermal synthesis. The activation of the reactions was made with a large-band of microwave frequencies pulse and a pulsatory regim of power, in a patented device for microwave treatment, conceived and built-up at INCDTIM. This new microwave technique proved to be a viable alternative to the conventional heating or microwave irradiation solvothermal synthesis. It is greener, faster and with lower power cosumption than convective heating solvothermal method. In contrast to the microwave-assisted solvothermal synthesis, our method is safer because it does not involve the heating of a closed bottle containing nitrates and volatile solvents.

Poster T3-5

H_2O_2 electrocatalytic reduction at carbon paste electrodes modified with Fe doped carbon aerogel

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Abstract. A new electrode material based on carbon paste electrodes (CPEs) modified with Fe doped carbon aerogel (Fe-CA) was used for H_2O_2 electrocatalytic reduction. Fe-CA have been prepared by sol–gel polymerization of formaldehyde with potassium salt of 2,4-dihydroxybenzoic acid, followed by K^+-exchange with Fe(II) ions from an aqueous solution of $Fe(OAc)_2$, and subsequent supercritical drying with CO_2. Carbonization at 1050°C, under an inert atmosphere, transforms the metal ion doped organic aerogels into metal and/or metal oxide nanoparticles-doped carbon aerogels. Surface area, pore size distribution, and pore volume were estimated by using N_2 adsorption/desorption isotherms with Brunauer– Emmett–Teller (BET) and Barrett–Joyner–Halenda (BJH) calculation methods. Phase identification and mean crystallite size evaluation were performed by analyzing the X-ray diffraction patterns. Fe-CA elemental analyses and TEM characterization were also performed. Basic electrochemistry of Fe-CA and its ability to catalyse the electroreduction of H_2O_2 have been investigated by cyclic voltammetry, performed in different experimental conditions (pH, potential scan rate, H_2O_2 concentration). The electroanalytical parameters of the new electrode recommend it as a stable, sensitive and reproducible sensor for H_2O_2 amperometric detection.

Poster T3-6

Wet air oxidation of phenol using copper doped carbon aerogel and xerogel as catalysts

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Abstract. Copper doped carbon aerogel and xerogel have been prepared by sol-gel polymerization of formaldehyde with potassium salt of 2,4-dihydroxybenzoic acid, followed by K^+-exchange with Cu(II) ions from an aqueous $Cu(NO_3)_2$ solution and subsequent drying realized either in supercritical conditions with CO_2 when copper doped organic aerogel was obtained or normal conditions when copper doped organic xerogel was obtained. Further pyrolysis at 750°C, under an inert atmosphere, transforms Cu ion doped organic aerogel and xerogel into Cu nanoparticles-doped carbon aerogel and xerogel (Cu-CA, Cu-CX). Resulted catalyst samples were investigated by nitrogen adsorption, TEM, X-ray diffraction, elemental analysis, etc. Cu-CA and Cu-CX catalysts were tested in the wet air oxidation process (CWAO) of phenol in aqueous solution. CWAO process was conducted in a thermostated batch reactor with a continuous feed of air from an air compressor at the desired flow rate. Various reaction parameters (oxygen flow rate, temperature, catalyst quantity, solution pH, phenol concentration) were tested. Reaction was followed using total organic carbon analysis (TOC).

Poster T3-7

Applying of Isoconversional Analysis to calorimetric data on the gel melting

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Abstract. As other polymer gels, gelatin gels are soft solids or, in other words, are polymer solutions that lost their ability to flow because of cross linking of polymer chains. Structurally, gelatin gels present an infinite network whose junctions are held by multiple hydrogen bonds. Gelatin gels have found numerous applications as food, pharmaceutical, cosmetic, photographic and other materials. Yet another novel application is in the area of tissue engineering materials that combine gelatin and various inorganic materials. The present study is concerned with thermal stability of gelatin gels that is defined as their resistance to melting or, in other words, to the thermally stimulated transition from gel to sol. The both sol-gel and gel-sol transitions were followed by regular (Mettler-Toledo DSC 823e) and stochastically modulated multi-frequency DSC (TOPEM® by Mettler-Toledo). The DSC data have been treated by using an advanced isoconversional method developed by Vyazovkin. The method allows one to reveal a variation in the effective activation energy (E_α) with the extent of conversion (α). It has been discovered that an increase in the concentration of gelatin solutions causes an increase in the energy barrier to melting of non-isothernally prepared gels.

Poster T3-8

Spectroscopic investigation of hemoglobin adsorbed onto gold nanoparticles

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Abstract. The adsorption of horse hemoglobin onto the surface of gold nanoparticles was studied using Uv-vis and fluorescence spectroscopy. The Soret band of hemoglobin in the presence of gold nanoparticles does not show significant changes, which proves that the protein retains its biological function. There’s a blue shift in the absorption band of gold nanoparticles, due to the attachment of hemoglobin molecules. Gold nanoparticles quench the fluorescence emission of tryptofan residues in the structure of hemoglobin. The Stern-Volmer quenching constant, the binding constant and the number of binding sites were also calculated.

Poster T3-9

Structural and microstructural of investigation of $Cd_xZn_{1-x}In_2S_4$ photocatalyst for solar hydrogen production

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Abstract. In recent years, photoelectrochemical water splitting for hydrogen production using solar energy has gained much attention. Using this method, intermittent solar radiation, which is unstorable, can be converted to chemical energy of hydrogen fuel, which is stable, clean, and storable. Therefore, the development of visible-light active photocatalysts with high efficiency is an urgent and important issue. Ternary chalcogenide semiconductors type $II\text{-}III_2\text{-}VI_4$ and their solid solutions are potential photocatalysts for application to photocatalytic hydrogen production due to their suitable properties such as high absorption in the visible region, appropriate flatband potential and good stability in aqueous sulfide solutions during irradiation. In this work, an X-ray diffraction based structural and microstructural study of chalcogenide semiconductors type $Cd_xZn_{1-x}In_2S_4$ ($0 \leq x \leq 1$) is reported. The investigated powder samples were synthesized by a hydrothermal technique, using a teflon lined closed autoclave with self-generated pressure, at 180^oC for 20 hours. Rietveld method based on pseudo-Voigt profile fitting function was applied to perform a simultaneous refinement of X-ray diffraction patterns concerning both material structure and microstructure. The Rietveld refinement of the X-ray diffraction data has been done using the the PowderCell, MAUD and FullProf softwares.

Poster T3-10

Hydrogen production by ethanol steam reforming on Ni/oxide catalysts

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Abstract. Hydrogen production from bio-fuels as bio-ethanol provides significant environmental benefits since the resulted CO_2 is consumed again for biomass growth, offering a carbon dioxide neutral energy source. In the actual conditions of increasing energy demand and atmosphere pollution, clean produced hydrogen can be an alternative option for a clean energy vector. In this paper we present the results obtained in hydrogen production by steam reforming of ethanol using nickel catalysts. Although Ni is not the most active catalyst for this process, economically is the most attractive one, due to the high price and low availability of noble metals. Ni was dispersed on several oxides: MgO, ZrO_2, Al_2O_3, Cr_2O_3, SiO_2 with a target metal concentration of 10 wt.% using impregnation method. The catalysts were characterized using several techniques: N_2 adsorption desorption isotherms to determine total surface area and porosity, XRD to determine oxide cristallinity and Ni crystallite size, TPR to determine NiO reducibility and its interaction with support. Each catalyst was tested in steam reforming of ethanol at temperatures ranging from 150 to 350°C, at atmospheric pressure and a ethanol : steam ratio of 1:10. The ethanol conversion and catalyst selectivity for H_2 depend on the support nature. The best results were obtained with Ni/ZrO_2 catalyst.

Poster T3-11

Laser induced silver substrate for SERS detection in separation methods

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Abstract. Development of Surface-enhanced Raman scattering (SERS) sensing approaches represents a goal for many research groups. This general aim brings about a lot of interesting new concepts and ideas whose success and impact may be judged over the years by their implementation in commercial instrumentation. SERS has the potential of a molecular specific, high sensitive detection method. Thus, it could be more advantageous compared to conventional UV-Vis absorbance or fluorescence used routinely for detection in chromatographic separation methods, like LC and TLC, as well as in capillary electrophoresis (CE). In most attempts described in the literature silver colloids are used as SERS substrate, even of major inconveniences. Here we propose a laser induced silver substrate for the Raman enhancement, prepared in-situ in the detection window. The small area of the prepared silver spot allows adsorption and desorption of analyte molecules to, or from the silver surface, without occurrence of perturbing memory effects during the SERS detection in a flow approach. Thus, due to the advantages of the proposed substrate, SERS detection was successfully implemented for CE and also a sequential multianalyte detection is shown by using the same silver substrate. The in-situ prepared silver substrate represents a valuable alternative to metal colloids, for SERS detection in flow systems.

Poster T3-12

Interaction of silver nanoparticles with some biomolecules

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Abstract. Silver nanoparticles were synthesized and characterized by UV-Vis spectroscopy, transmission electron microscopy and atomic force microscopy (AFM). The average diameter of silver particles was about 10 nm ± 1 nm. The interaction of silver nanoparticles with various biomolecules was monitored using UV-Vis spectroscopy, AFM and TEM. A strong interaction of silver nanoparticles with biomolecules of anesthetics has been noticed, resulting in a stable self-assembly of nanoparticles. These results offer the premises for further applications in nanotechnology and nanomedicine.

Poster T3-13

Thermodynamic Characterization of Mixed Lipids at the Air-Water Interface

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Abstract. Self assemblies of mixed cholesterol (CHO) and dimyristoyl phosphatidyl choline (DMPC) monolayers spread at the air/water interface were prepared and investigated by compression isotherms using Langmuir technique (LT). Surface excess Gibbs energy of mixing was calculated for different compositions of the DMPC-cholesterol mixed films. By means of the Langmuir-Blodgett technique (LBT), these self assemblies were transferred on solid support (e.g. glass optically polished) and were characterized by atomic force microscopy (AFM) imaging technique. This investigation demonstrates that rather strong interactions between these lipid molecules, DMPC and CHO molecules, lead to well defined two-dimensional stable nanostructures characterised by low surface roughness. These lipid self assemblies could have practical applications for biosensors fabrication. They also occur within natural membranes representing the lipid matrix where in vivo the protein molecules are embedded or adsorbed.

Poster T3-14

Structural and magnetic properties of some gadolinium-zinc-borate glasses and glass ceramics

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Abstract. X-ray diffraction (XRD), electron paramagnetic resonance (EPR) and magnetic susceptibility measurements have been employed to investigate the samples from the $(Gd_2O_3)_x\cdot(B_2O_3)_{(60-x)}\cdot(ZnO)_{40}$ $(0 \leq x \leq 20$ mol%) system. The XRD pattern for the prepared samples shows that the vitreous phase is present only for $x \leq 15$ mol%. For the samples containing 20 mol% Gd_2O_3 the presence of a unique crystalline phase, $GdBO_3$, embedded in an amorphous matrix was evidenced. In this case the XRD patterns show the presence of nanometer crystals (64 nm) in a glassy matrix. The EPR spectra of the studied samples exhibit three important features with effective g-values of ≈ 6, 2.8, 2.0 and a weaker feature at $g \approx 4.8$. For low Gd_2O_3 contents ($x < 3$ mol%), the EPR spectra have the typical ''U''-type shape. For higher contents of Gd_2O_3 ($x \geq 3$ mol%), the spectral features are broadened and finally are dominated by a single broad absorption line located at $g \approx 2.0$. This broad EPR line is associated to the Gd^{3+} ions present predominantly as clustered species. Magnetic susceptibility data show that for $x > 1$ mol% the Gd^{3+} ions are predominantly clustered and are coupled through antiferromagnetic exchange interaction.

Poster T3-15

Oxidation of atenolol using a glassy carbon electrode modified with gold nanoparticles

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Abstract. The study of atenolol oxidation by various electrochemical techniques may provide valuable information about the redox process of this molecule. Amino acid layers/AuNPs multicomponent structure was used to modify the surface of a glassy carbon electrode and then to study atenolol oxidation by Linear Sweep Voltammetry and Electrochemical Impedance Spectroscopy. The chosen design allows for the detection of atenolol oxidation peak at a considerably lower potential (+0.65 V/SCE) in comparison with previously reported results. The linear detection range for atenolol was between 10^{-5} -10^{-3} M and the detection limit was found to be of 3,9 x 10^{-7} M. Such findings could be incorporated in highly sensitive detection technologies of various biological or chemical compounds and molecules.

Poster T3-16

EPR characterization of glass system xMn_(1-x)·[45ZnO·55B_2O_3]

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Abstract. Glasses system xMn_(1-x) [45ZnO·55B_2O_3] (0.5 %mol ≤ x ≥ 40 %mol) have been prepared by melting at 1200 °C and rapidly cooling at room temperature. The obtained samples were subjected to an additional thermal treatment in order to relax the glass structure and to improve the local order. Electron Paramagnetic Resonance (EPR) spectroscopy is a very sensitive technique for the investigation of the TM ionic states and their local environments and interactions. In the present contribution, we report an EPR investigation of xMn_(1-x) [45ZnO·55B_2O_3] system.The local structure in the investigated glasses was revealed by means of EPR using Mn^{2+} ions as paramagnetic probes. The EPR spectra present two resonance absorption lines characteristic to Mn^{2+} ions centered at g_{eff} ~ 2.0, for $0 < x \leq 35$ mol% and g_{eff} ~ 4.3, for $0 < x \leq 1$ mol%. The variation of the EPR parameters, the intensity and line-width of these absorption lines, with manganese ions composition has been studied.

Poster T3-17

Investigation of carbamazepine oxidation using modified gold electrode

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Abstract. Carbamazepine is currently considered as one of the emerging pollutants in ground and surface water, therefore its accurate determination by fast and reliable methods is highly desirable. Recent studies found that carbamazepine is persistent and its removal efficiencies by the wastewater treatment plants (WWTPs) are below 10%. The employment of electrochemical techniques for detection of carbamazepine is a valuable alternative to the more laborious methods generally used, like liquid chromatographic methods. The work presented here aims to study the oxidation of carbamazepine, taking advantage of the electrocatalytic properties of graphene modified gold surface. Such nanostructured surface represents an alternative to other analytical methods, being suitable for fast and inexpensive determinations. The morphological characteristics of graphene-gold surface were investigated by Atomic Force Microscopy (AFM). In addition, we employed Cyclic Voltammetry (CV), Linear Sweep Voltammetry (LSV) and Electrochemical Impedance Spectroscopy (EIS) to characterize the electrocatalytic properties of graphene-gold electrode.

Poster T3-18

Lipoic acid and beta-cyclodextrin supramolecular associations

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Abstract. Supramolecular associations, named also inclusion complexes, of lipoic acid and beta-cyclodextrin, are obtained by different preparation methods: kneading, co-precipitation and freeze-drying. The supramolecular associations are investigated by advanced spectroscopic methods (such as FTIR), X-ray diffraction methods (XRD) and differential scanning calorimetric measurements (DSC) to evidence their formation. The crystalline structure of these complexes was also determined from a combination of X-ray diffraction data with molecular mechanics calculations. Molecular modeling (MM+ molecular mechanics) shows the spatial architectures of supramolecular associations at the optimum molar ratio in good agreement with experimental data. To provide insight into the self assembly formation of these compounds, the self-assembled films were deposited, on different solid supports, such as glass and mica, and investigated by AFM and SEM. The morphology of self assembled films formed from lipoic acid and beta-cyclodextrin revealed the films nanostructure. These results are in substantial agreement with the experimental and thermodynamic data gained about supramolecular associations of lipoic acid and beta-cyclodextrin. These findings may constitute a direct contribution to the molecular encapsulation of lipoic acid into beta-cyclodextrin. The encapsulation might improve lipoic acid stability and bioavailability, taking into account that lipoic acid is an important nutrition supplement used in the treatment of some blood disorders and cancer.

Poster T3-19

The influence of Al and Gd doping on structural, microstructural, optical and EPR properties of ZnO thin films

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Abstract. Zinc oxide (ZnO) is known for its many potential applications such as thin films transistors, window materials in solar cells, laser diodes, transparent conductive contacts, optoelectronic and piezoelelectric applications and many others. The undoped ZnO contains a choice of defects which will influence the luminescence properties of ZnO. By introducing Al and Gd as a dopant, it is expected that optical and electrical properties change.The ZnO, Al:ZnO and Gd:Al:ZnO thin films were deposited on glass substrates by RF magnetron sputtering technique. It was used 99.999% pure ZnO, 2 at.%Al_2O_3 ($ZnAl_{2\%}O$) and 1.5 at.%Al_2O_3 0.5 at. Gd_2O_3 ($ZnGd_{0.5\%}Al_{1.5\%}O$) ceramic targets, all fabricated by solid state reaction method. The surface morphology characterized by atomic force microscopy (AFM) in tapping mode, shows the presence of columnar morphologies with increased roughness for doped Al and Gd thin films. X-ray diffraction (XRD) revealed that ZnO doped with Al and Gd enhanced the crystallinity of ZnO thin films. Optical transmittance spectra, taken at room temperature in air, showed that the optical edge of ZnO is shifted to a shorter wavelength with the increasing of Al and Gd dopants. The influence of Al doping was studied by electrical resistivity measurement function of temperature. The low resistivity was observed for 2% Al doped ZnO films. Local magnetic interactions aroung Gd ion were investigated by EPR measurements.

Poster T3-20

Magnetic resonance investigations of $Zn_{1-X}Fe_XO$ nanopowders

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Abstract. ZnO is an attractive system for quite a wide variety practical applications, being a chemically stable oxide semiconductor. It has been shown that Fe doping produces ferromagnetic semiconductor at room temperature. This material, therefore, has the potential for use in spintronic devices such as spin transistors, spin light emiting diodes, very high density nonvolatile semiconductor memory and optical emitters. It is believed that oxygen vacancies and substitutional incorporation are important to produce ferromagnetism in semiconductor oxide doped with transition metal ions. The present paper reports detailed electron paramagnetic resonance investigations (EPR) of the samples in order to investigate how Fe ions are incorporated into the ZnO lattice and their interaction with environment.

X-band electron paramagnetic resonance (EPR) studies of Fe^{3+} ions in $Zn_{1-x}Fe_xO$ powders with X = 1%, 3%, 5% is reported. These samples are interesting to investigate as Fe doping produce ferromagnetism in ZnO, making a promising ferromagnetic semiconductor at room temperature.

Poster T3-21

TiO_2/Methylcellulose nanocomposite films for photocatalytic applications

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Abstract. TiO_2/methylcellulose (MeC) nanocomposite films were obtained by wet-chemical techniques using MeC and/or additives (distillated water, acetylacetone, polyethyleneglycol and Triton X) as a dispersant, deposition the colloidal suspensions by spin-coating on ITO glass and followed by a heat-treatment. The effect of MeC and additives on dispersion TiO_2 nanoparticles, structural and morphological properties (FTIR microscopy and X-ray diffraction), optoelectronic properties (UV-VIS absorption spectroscopy and spectrofluorimetry) and mechanical integrity (wet technique adhesion test) of the TiO_2 films were investigated. The composite films with methylcellulose have much rougher surface than films made without methylcellulose, good film integrity and a superior adhesion, without diminishing the photocatalytic activity. The results of these experiments promote these nanocomposite films as interesting candidate for practical catalytic applications in the field of photocatalytic degradation of organic pollutants.

Poster T3-22

Structural and microstructural characterization of nanocrystalline $(CuIn)_{0.1}Zn_{1.8}S_2$ photocatalysts for solar hydrogen production

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Abstract. Semiconductor photocatalyis has been applied to a variety of problems of environmental interest in addition to water and air purification and for the photo splitting of water to produce hydrogen gas. A series of ZnS structure type photocatalysts were synthesized by a hydrothermal method. The hydrothermal synthesis technique of chalcogenide $Zn_{2x}(CuIn)_{1-x}S_2$ semiconductors was performed in a teflon lined closed autoclave with self-generated pressure. We report here an X-ray diffraction investigation using Rietveld method for structural and microstructural study of chalcogenide $Zn_{1.8}(CuIn)_{0.1}S_2$ photocatalysts, obtained under different hydrothermal conditions.

Poster T3-23

Structural characterization of ZnS thin films by X-ray scattering

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Abstract. Studies of sulphide thin films are quite important because of their possible technological applications. Among the various sulphides, zinc sulphide (ZnS) have been extensively studied from both experimental and theoretical points of view. The interest for these materials is based on their potential applications, in optoelectronic devices such as light emitting diodes, optical filters and luminescent nanocomposites. ZnS thin films were prepared by chemical bath deposition from aqueous solutions of zinc acetate (for Zn source), thiourea (for S source) in a hot basic medium using and sodium citrate. In the present work we are interested in studies concerning the local structure of amorphous ZnS thin films by using wide-angle X-ray scattering (WAXS) method. The effect of the thermal treatment on the amorphous thin film of ZnS thin films structure it is also evidenced. After the formulation of hypotheses on the local order of the chalcogenide system has been enounced, the radial distribution function (RDF) analysis was done and the atom co-ordinations were determined. The radius of the first coordination spheres was evaluated by using the correlation function g(r) resulted from the X-ray scattering measurements.

Poster T3-24

TiO_2 thin film deposition by chemical methods

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Abstract. Mesoporous nanocrystalline TiO_2 dye sensitized solar cells was obtained by the sol-gel process in an aqueous solution using the titanium diethanolamine complex as the precursor and the spin coating technique to obtain TiO_2 films on ITO (Indium Tin Oxide) glass substrates.

TG – DTA, RES, BET, FT-IR, UV – VIS, SEM, Raman spectroscopy, X-ray diffraction techniques and cyclic voltammetry measurements, have been used to investigate the chemical and physical changes during the sol - gel process and the characteristics of the TiO_2 powder precursor.

In this paper, we report the preparation of TiO_2 films by sol – gel technique based on precursor solution employing diethanolamine as the stabilizing agent to prevent precipitation of titanium butoxide ($Ti(OC_4H_9)_4$) by ethanol. The stabilizing action of diethanolamine is an outcome of its chelate forming ability with the alkoxides. Diethanolamine interacts with titanium alkoxide as a tridentate ligand.

Poster T3-25

Electrochemical behavior of gold nanoparticles functionalized with leucine-modified carbon paste electrode

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Abstract. Gold nanoparticles (GNP) are intensively studied due to their interesting optical, electronic, catalytic and biological applications. GNP have demonstrated to be very appropriate for the development of modified electrodes. Thus, many biological molecules including enzymes, antibodies, nucleic acids and aminoacids are physically adsorbed on gold nanoparticles without loss of their biological activity. Colloidal gold-modified electrodes have been prepared using glassy carbon, metal Au and carbon paste as electrode substrates. GNP have also demonstrate to constitute useful interfaces for the electrocatalysis of redox processes of molecules such as H_2O_2, O_2 or NADH involved in many significant biochemical reactions. A new composite electrode material consisting of GNP synthesized by citrate reduction and functionalizated with L-leucine was incorporate in carbon paste (CP) and characterized. The electrochemical behavior of carbon paste electrodes GNP-LEU-CPE has been investigated at various pH values and potential scan rates using cyclic voltammetry (CV) measurements. Finally, the electrocatalytic activity of the modified electrodes GNP-CPE and GNP-LEU-CPE toward H_2O_2 reduction were investigated. The results demonstrate that functionalized GNP plays an important role in the study of electrochemical sensors and development of promising electrocatalytic or biosensing applications.

Section T4:

Isotopic materials and processes

Oral T4-1

Reduction of U(VI) adsorbed on anion exchange resin with V(III) in acid solution

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Abstract The results concerning the reduction of U(VI) adsorbed on anion exchange resin as uranyl chloro complexes and sulfate complexes with V(III) in HCl and H_2SO_4 solution are presented. The reduction of uranyl sulfate adsorbed on anion exchange resin ($UO_2SO_{4(R)}$) in 0.05 M sulfuric acid was carried out, the reaction rate being first order with respect to both concentrations: $[U(VI)_{(R)}]$ and [V(III)]. From Arrhenius plot the activation parameters of the reaction between $U(VI)_{(R)}$ and V(III) in sulfuric acid solution were determined: $E_a = 34.9 \pm 0.9$ kJ/mol; $\Delta H^{\neq} = 35.5 \pm 0.9$ kJ/mol and $\Delta S^{\neq} = - 165.7 \pm 3$ J/K·mol. The reduction reaction rate makes possible the utilization of this reaction for displacement of the uranium adsorption band in a ^{235}U separation column packed with anion exchange resin.

Oral T4-2

Isotopic ratios applications in the detection of illegal watering of wines and fruit juices

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Abstract. In the last years, a growing number of research articles detailing the use of natural abundance isotope variations as a tool in the fight against fraud in the food industry have been published. One of the greatest limitations to the applications of the technique in origin assignation is the lack of large databases of isotopic abundance in food items. The interpretation of such analysis requires a sufficient number of data for authentic wines and juices of the same seasonal and regional origin, especially since the isotopic parameters of these show remarkable variability depending on climatologically factors.

In this work, the applications of the H, C, O stable isotope ratios in the assessment of watering in beverages, such as wine and fruit juices, commercialized on Romanian market are presented and discussed.

Oral T4-3

A simplified mathematical model of the cryogenic distillation with application to the (^{13}C) isotope separation column

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Abstract. The isotope (^{13}C) has a widespread application in many fields such as chemistry, physics, medicine, etc. To obtain a high concentration in isotope of interest, in our case (^{13}C), it is used the method of cryogenic distillation of carbon monoxide (CO) which is based on the difference between the vapour pressure ($^{12}C^{16}O$) and ($^{13}C^{16}O$) at the temperature of liquid nitrogen. Isotope separation column, used to obtain the isotope (^{13}C), is a complex installation, with many inputs and outputs, rather difficult to control. Due to this reason, from the point of view of automation, it is needed a simplified mathematical model. This model can be determined only with some presumption and simplification assumptions. Using the physical laws, the hydrodynamic part of the process will be described by partial differential equations. The mass balance from the column will result other equations. In order to design a controller for the column, it is needed a transfer function or a state-space realization of the plant, which is the main contribution of the present work. Implementing this mathematical model will be the key element for describing and understanding the operation of the plant and for future development of process control strategies.

Oral T4-4

Separation of Am(III) from Eu(III) by extraction chromatographic technique using functional polymer gels with TPEN analogs

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Abstract. *N*,*N*,*N'*,*N'*-tetrakis(2-pyridylmethyl)ethylenediamine (TPEN) is one of the podand-type ligands with six nitrogen-donors and recognizes the slight difference in the softness between trivalent MA (minor actinides) and Ln (lanthanides). A new chromatographic agent, in which TPEN was immobilized chemically in a polymer gel, were produced and were applied to the separation of MA from Ln. *N*,*N*,*N'*,*N'*-tetrakis-(4-propenyloxy-2-pyridylmethyl)ethylenediamine (TPPEN), in which propenyloxy groups were introduced to 4 pyridine rings of TPEN, was used as a cross-linker of acrylic monomers and some polymer gels were synthesized by the copolymerization of TPPEN and acrylic monomers, such as *N*-isopropylacrylamide (NIPA), acrylic acid (AAc), methyl methacrylate (MMA), and *N*,*N*-dimethylacrylamide (DMAAm). The adsorption of ^{241}Am(III) (MA) and ^{152}Eu(III) (Ln) into these gels were tested. In the pH range of 4 to 5, NIPA-TPPEN gel and DMAAm-TPPEN gel showed high separation factors of Am(III) over Eu(III) ($SF_{\mathrm{Am/Eu}}$), which were evaluated to be 26 and 18, respectively. These values are sufficient for the chromatographic separation of MA. The adsorbed Am(III) was recovered easily in an acidic eluent at pH 2.

Poster T4-1

Catalytic reduction of sulfuric acid to sulfur dioxide

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Abstract. The reduction reaction of sulfuric acid to sulfur dioxide is included in thermochemical cycles for hydrogen production from water at lower temperature (<1000°C) than that of the direct thermal splitting of water (>2200°C). Conversion of H_2SO_4, resulted as byproduct in ^{15}N separation by isotope exchange method in Nitrox system, to SO_2, is the way in which sulfur dioxide can be recycled in the ^{15}N production plant. The reduction of H_2SO_4 to SO_2 occurs with a relativelly good efficiency only at high temperatures in the presence of catalysts. Some experimental results, regarding conversion of sulfuric acid (96%) to sulfur dioxide and oxygen, are reported in this work, the reduction being performed at 800 - 900°C and atmospheric pressure in a tubular quartz reactor. The following commercial catalysts were tested: Pd / Al_2O_3 (5% and 0.5% Pd), Pt / Al_2O_3 (0.1% Pt) and Fe_2O_3. X-Ray diffraction analyses and SEM were used in order to characterize the fresh and spent catalysts. The highest catalytic activity was determined for Pd (5%) / Al_2O_3, a conversion of 80% being obtained for 5 hours at 9 ml/h flow rate of 96% H_2SO_4. In the same experimental conditions a conversion of 64% was determined for Pd (0.5%) / Al_2O_3 and Pt (0.1%) / Al_2O_3. In the case of Fe_2O_3 a less expensive catalyst, a conversion of 61% for about 50 hours was obtained.

Poster T4-2

The study of the local sources of CO_2 using stable isotopes

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Abstract. The main goal of this study is to provide the scientific data and analysis to reduce contributions to atmospheric carbon dioxide. To achieve this goal we have studied the mechanisms controlling carbon release by gasoline combustion, natural gas combustion and biogenic respiration of plants on CO_2 mixing ratio in an urban area of Cluj Napoca city, Romania. We have identified the sources of the carbon dioxide in this area taking the advantage of the individual “fingerprint”, i.e. stable isotope signature of each source. We measured the CO_2 concentration and the isotopic composition of ^{13}C in CO_2, and we constructed the Keeling plots to determine the nature of the sources of CO_2 in the area. We have found the main source in the area is anthropogenic and the biogenic sources can be neglect.

Poster T4-3

The use of isotope ratios for vegetable oils authentication

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Abstract. Adulteration of a product consists in making it impure by fraudulent addition of a foreign or inferior substance. The result is either an alteration of the product and of its quality or a falsification. The falsification is a voluntary act with the intention of abuse. The falsification may be more or less sophisticated and its sophistication as well as its costs increases with the improvement of analytical methods. In this study 22 vegetable oils (olive, sunflower, palm, maize) commercialized on Romanian market were investigated by mean of $\delta^{13}C$ in bulk oil and the obtained results were compared with those reported in literature in order to check the labeling of these products. The obtained results were in the range of the mean values found in the literature for these types of oils, thus providing their accurate labeling.

Poster T4-4

Multielement and stable isotope determinations in some Transylvanian fruit juices

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Abstract. Different soils have different quality and quantity of mineral elements. Major and trace elements composition of fruits is a distorted reflection of the element composition of the soil in which the plant grows. Soil also contains potentially toxic elements (i.e. heavy metals or trace elements). Heavy metals in soil are mostly bound by soil particles and are therefore not very mobile. Therefore they can accumulate and persist in soils for long period. At certain concentrations in plants heavy metals can be harmful for human health. Inductively coupled plasma-mass spectrometry (ICP-MS) is a multielement technique suitable for detailed characterization of the elemental composition of numerous samples, including soils and juices. In this work, multielement composition of the chain soil-leaf-fruit was realized by ICP-MS technique. These data were correlated with $\delta^{13}C$ of the fruit pulp in order to assess the geographical fingerprint.

Poster T4-5

The CO_2 desorption from carbamate solutions for the ^{13}C separation by chemical exchange

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Abstract. The CO_2 desorption from amine solutions in non-aqueous solvents is of major importance for isotopic exchange. A series of experiments were carried out to in order to set up the optimal conditions for the CO_2 desorption. For this purpose, a laboratory- scale installation for separation based on chemical exchange was designed and used. The decomposition of the carbamate solution was mostly made in the desorber and completed in the boiler. Two different-length desorbers were used, at different temperatures and liquid flows of the amine-non-aqueous solvent solutions. The residual CO_2 was determined by using volumetric and gas-chromatographic methods. These results can be used for ^{13}C separation, reducing the unwanted isotopic recombination to the minimum.

Poster T4-6

Boiler DC power control for ^{13}C separation column

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Abstract. The cryogenic ^{13}C separation column load is decided in the first line by the thermal power dissipated in boiler, electrically heated. The actual open loop control by measuring the resistor voltage (UR) present some drawbacks like: non-linear input/output relationship, control with bias by variation of the heating resistor parameters and important errors by power line changes. In order to avoid any electro-magnetic interference (EMI) the solution of the DC supply is chosen. The actual solution is based on a real DC power transducer (0-8VDC) for (0-110W) and the closed loop structure using the pulse-width modulation principle. The mode of operation and general performance on various power resistors, some of them similar to the resistor from boiler, are also presented.

Poster T4-7

The use of stable isotopes in quantitative determinations of exogenous water in wines

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Abstract. The application of oxygen isotope ratios analysis to wine water according to EU regulation no. 822/97 to determine wine's origin and also, the possible water addition to wines, in order to obtain an illegally economical profit, gained great importance in wines authenticity control. In the natural cycle of water isotopic fractionation occurs during water evaporation which depleted in heavy isotopes are observed in the vapour over liquid. A similar fractionation occurs if water evapotranspiration from plants, leading to high isotope enrichment of stable isotopes of water content in plants compared with meteoric water. This is the principle behind the detection of exogenous water from wines.

This work presents the way in which, by using isotopic fingerprint, the percent of exogenous water from wines can be precisely determined.

Poster T4-8

The kinetics reduction of U(VI) adsorbed on anionit with Ti(III), in HCl solution

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Abstract. In the process of ^{235}U enrichment by chemical exchange in U(VI)$_{(R)}$ - U(IV)$_{(S)}$ on anion exchange resin, the displacement of uranium band in the separation column is done by using a solution of $TiCl_3$ as reducing agent and a solution of $FeCl_3$ as oxidant agent. At the rear boundary of uranium band, uranyl ions, adsorbed on resin as chlorocomplexes, are reduced to U(IV) and eluted to the aqueous phase, which flows down through the uranium adsorption band. In the zone of uranium band the isotope exchange reaction takes place between uranium species in the moving phase of solution and the uranium species in the anion exchange resin. In order to have a sharp boundary between uranium adsorption band and the reducing agent zone the reaction between U(VI)$_{(R)}$ and Ti(III)$_{(S)}$ should be rapid and complete. The results concerning the reduction of U(VI)$_{(R)}$ adsorbed on anion exchange resin as uranyl chlorocomplexes and $TiCl_3$ in HCl 5M solution are presented. The kinetic measurements were carried out by putting into contact 1 g anion exchange resin Dowex – Marathon, charged with UO_2Cl_2 with $TiCl_3$ solution in 5M HCl. The experimental data showed a global order two of the reaction between U(VI)$_{(R)}$ and Ti(III)$_{(S)}$. Two more sets of experiments were done in order to establish the reaction order with respect to each reactant. The experimental data at room temperature showed that the reaction rate is first order with respect to the both concentrations: [U(VI)$_{(R)}$] and [Ti(III)$_{(S)}$], the rate makes possible the utilization of this reaction for elution of the uranium adsorption band in a ^{235}U enrichment column with anion exchange resin.

Poster T4-9

Deuterium isotopic characterization of long-term precipitation water

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Abstract. Within the water cycle, temperature at the location where vapors condense to precipitation has been heralded as primary controlling factor in the fractionation of stable isotope in precipitations. Because atmospheric temperature dictates the pressure of aqueous vapor in the atmosphere and pressure controls the isotopic composition of atmospheric water vapors, changes in the temperature dictate different rates of fractionation. The studies related to water transport in the water natural cycle are primary based on isotopic analysis of precipitations, using as natural tracers the stable isotopes of hydrogen and oxygen. The advantage to use the stable isotopes of water as tracers in earth and life sciences resides in the fact that they are available in the nature, they are not pollutant, non-invasive, space and time unlimited in use and can be investigated from micro- to macroscale. The strong link between long-term monthly mean values of the local surface air temperature and the deuterium abundance of precipitation fallen over Cluj-Napoca, Romania in the time period 1975-2010 was evidenced is used for the determination of deuterium content in precipitation from another site from Romania with reasonable confidence. These findings are necessary for studies of groundwater and water movement in wetland.

Poster T4-10

The use of stable isotope ratios and trace elements in quality control of fruit juices

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Abstract. In the last years, a growing number of research articles detailing the use of natural abundance isotope variations and elemental concentration as geographic “tracers” to determine the provenance of food have been published. These investigations exploit the systematic global variations of stable hydrogen, oxygen and carbon isotope ratios in combination with elemental concentrations. The elemental content of plants and also their isotopic ratios content is mainly related to the geological and pedoclimatic characteristic of the site of growth. One of the greatest limitations to the applications of the technique in origin assignation is the lack of large databases of isotopic abundance in food items. The interpretation of such analysis requires a sufficient number of data for authentic juices of the same seasonal and regional origin, especially since the isotopic parameters of fruit juices show remarkable variability depending on climatologically factors.

In this work, H, C, O stable isotope ratios and the content of 9 elements (Cu, Cr, Ni, Zn, Pb, Co, As, Cd and U) of 12 single strength juices are presented and discussed.

Poster T4-11

Preliminaries on the influence of catalysts upon the ^{13}C enrichment by chemical exchange CO_2 – carbamate method

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Abstract. The main problem of the ^{13}C separation by chemical exchange CO_2 – carbamate is the low isotopic exchange rate that leads to the increase of both the HETP and the steady state reaching time of the isotope separation plants. The present paper analyses the influence and the limits of using of catalysts on this type of isotope separation process. Experiments were performed both for amine – polar and non polar solvents. For amine-polar solvent system $CuCl_2$ or $NiCl_2$ produced the best results. The experiments show that with optimal catalyst concentrations, the isotope separation is up to 24% increased in an amine-polar solvent system. The catalysts also influence the separation in amine-non polar solvent system.

Authors index

Alberst S Oral T2-1

Aldea N Poster T2-8; Oral T3-1; Oral T3-7

Alder A C Poster T1-15

Almasan V Oral T2-3; Poster T3-10

Altucci C Poster T2-11

Aluas M Poster T1-25; Poster T1-30

Andersen J N Poster T1-11

Anghel S D Poster T2-12

Apetrei A Pl-5

Ardelean C Poster T3-2

Ardelean O Oral T2-4; Poster T2-2; Oral T3-4; Poster T3-1; Poster T3-4

Ardelean P Poster T3-2

Ardelean S Poster T3-3; Poster T3-17

Asandei A Pl-5

Ataman E Poster T1-11

Avram V Oral T1-3; Poster T1-1; Poster T1-15; Poster T1-19; Poster T1-26

Axente D Oral T4-1; Poster T4-1; Poster T4-8

Bakatula E Oral T3-8

Balazs Z Poster T3-2

Baldea A Poster T4-5; Poster T4-6; Poster T4-11

Balla A Oral T4-1; Poster T4-1; Poster T4-8

Banica R Poster T3-9; Poster T3-22

Barbu-Tudoran L	Poster T1-29
Bayot V	Pl-6
Beginn U	Pl-1
Bele C	Poster T1-14
Bende A	Oral T1-2; Poster T3-2
Beu T A	Pl-2
Biris A R	Pl-3; Oral T3-3; Poster T3-3; Poster T3-17; Poster T3-24
Biris A S	Pl-3; Oral T3-3; Poster T3-3
Biro L P	Pl-13
Blanita G	Oral T2-4; Poster T2-2; Oral T3-4; Poster T3-1; Poster T3-4
Bogdan D	Oral T3-5
Bogdan M	Poster T1-3; Poster T1-9; Poster T1-22
Bojita M	Poster T1-25
Bopp G	Pl-1
Boquet M L	Poster T1-11
Borodi Gh	Oral T1-2; Poster T1-4; Poster T1-8; Poster T1-13; Poster T1-21; Poster T1-25; Poster T3-14; Poster T3-18; Poster T4-1
Boros T	Oral T3-12
Bot A	Poster T2-6
Braga D	Oral T1-4
Bratu I	Oral T1-1; Oral T1-2; Poster T1-4; Poster T1-7; Poster T1-12; Poster T1-16; Poster T1-19; Poster T1-21; Poster T1-25; Poster T1-29; Oral T2-6; Poster T3-18; Poster T3-21; Poster T3-24; Poster T3-25
Brueser V	Oral T3-1
Buimaga-Iarinca L	Poster T1-10; Poster T1-29

Buling A	Pl-8
Calborean A	Poster T2-1
Canpean V	Poster T3-15; Poster T3-17
Cazac T	Poster T1-23
Chis V	Poster T1-18; Poster T2-1
Chvalun S N	Pl-1
Ciupa R	Poster T2-10
Coca-Podaru C	Oral T3-2
Coldea I	Oral T2-4; Poster T2-2; Oral T3-4; Poster T3-1; Poster T3-4
Copaciu F	Poster T1-27
Cotet L C	Poster T3-5; Poster T3-6
Craciunescu I	Oral T1-5; Oral T3-2; Oral T3-6; Oral T3-11
Cristea G	Oral T4-2; Poster T4-2; Poster T4-3; Poster T4-7
Cristian F	Oral T4-3
Culea E	Poster T2-3; Poster T3-14
Cuna S M	Oral T4-2; Poster T4-2
Dadarlat D	Poster T1-5; Poster T1-6; Poster T1-21
Daia C	Oral T3-2; Oral T3-12
Dan M	Poster T3-10
Danciu V	Poster T2-3; Poster T3-5; Poster T3-6
Darabont Al	Poster T3-20
David L	Poster T1-26
Dehelean A	Poster T1-31; Poster T1-32; Poster T2-3; Poster T2-13; Poster T4-4; Poster T4-10

Derks C Pl-8

Derviski E Pl-3; Oral T3-3; Poster T3-3

Desplanque L Pl-6

Dobrik G Pl-13

Dombi P Poster T2-5

Dordai E Poster T4-2

Dragan F Poster T1-7

Dranca I Poster T3-7

Dreve S Oral T1-2; Poster T3-2; Poster T3-21

Driver A J Oral T3-3

Dronca S Poster T4-5; Poster T4-11

Duclairoir F Poster T2-1

Dulf E H Oral T4-3; Poster T4-6

Faniel S Pl-6

Farcas F Oral T2-1

Feher I Poster T1-19; Poster T1-26

Festila C Oral T4-3; Poster T4-6

Filip C Poster T1-8; Poster T1-30

Filip X Poster T1-8; Poster T1-30

Floare C Poster T1-3; Poster T1-9; Poster T1-22

Fort C I Poster T3-5; Poster T3-6

Ganea M Poster T1-7

Garabagiu S Poster T3-8

Gheorghe N G Oral T3-7

Girbovan D	Poster T3-19
Giurgiu L M	Poster T3-20
Gligan M	Oral T4-3; Poster T4-5; Poster T4-11
Gluck P	Oral T2-2
Grajewski J	Poster T1-20
Grawronski J	Poster T1-20
Grepioni F	Oral T1-4
Grosan C	Poster T3-25
Hackens B	Pl-6
Hincu L	Poster T1-7
Hodisan T	Poster T1-16
Hodor I	Pl-4; Poster T4-5
Horovitz O	Poster T3-12; Poster T3-13
Hu D T	Oral T3-13
Huant S	Pl-6
Hwang C Y	Pl-13
Indrea E	Oral T3-8; Poster T3-2; Poster T3-9; Poster T3-21; Poster T3-22; Poster T3-23; Poster T3-24
Isvoranu C	Poster T1-11
Iuga C	Poster T1-25
Jitian S	Poster T1-12
Jumate N	Poster T1-21; Poster T4-1
Kacso I	Oral T1-1; Oral T1-2; Poster T1-21; Poster T1-25; Poster T3-18
Karsten S	Oral T3-11

Kebdani O	Oral T3-3
Knudsen J	Poster T1-11
Kolipaka K L	Oral T3-1
Kovacs K	Poster T2-5; Poster T2-11
Kovacs M H	Poster T1-32; Poster T2-13
Kuepper K	Pl-8
Lampronti G	Oral T1-4
Lazar M	Poster T1-16
Lazar M D	Oral T2-3; Poster T3-3; Poster T3-10; Poster T3-17
Leopold N	Poster T1-18; Poster T3-11
Leostean C	Oral T3-7; Oral T3-11
Liebscher J	Poster T2-4; Oral T3-6; Oral T3-11
Lung I	Poster T1-14; Poster T1-28
Lung R	Poster T3-14
Lupascu T	Poster T3-7
Luchian T	Pl-5
Lupu D	Oral T2-4; Poster T2-2; Oral T3-4; Poster T3-1; Poster T3-4
Macavei S	Oral T3-7
Magdas A D	Poster T1-31; Oral T4-2; Poster T4-2; Poster T4-3; Poster T4-4; Poster T4-7; Poster T4-10
Maicaneanu A	Poster T3-6
Maini L	Oral T1-4
Maldivi P	Poster T2-1
Marconti D	Poster T3-19

Marcu C	Oral T4-1; Poster T4-1; Poster T4-8
Marian I	Poster T3-24
Marincas O	Oral T1-3; Poster T1-15; Poster T1-19
Marinica O	Oral T3-12
Martins F	Pl-6
Marutoiu C	Oral T1-1; Poster T1-19
Marutoiu C	Poster T1-16; Poster T1-19
Marutoiu O F	Poster T1-16
Marutoiu V C	Oral T1-1
Matea C	Poster T1-14
Mereuta L	Pl-5
Mic M	Oral T1-5; Poster T1-17
Mihailescu Gh	Poster T3-2; Poster T3-8
Mihaly-Cosmuta A	Oral T3-8
Mihaly-Cosmuta L	Oral T3-8
Mihet M	Oral T2-3; Poster T3-10; Poster T3-24
Mircescu N E	Poster T1-18
Mirel V	Poster T1-32; Oral T2-3; Poster T4-2; Poster T4-3
Misan I	Oral T2-4; Poster T2-2; Oral T3-4; Poster T3-1; Poster T3-4
Mocanu A	Poster T3-12; Poster T3-13; Poster T3-18
Moisa C	Poster T1-7
Moldovan Z	Oral T1-1; Oral T1-3; Poster T1-1; Poster T1-15; Poster T1-19; Poster T1-26; Poster T1-31; Oral T2-6; Poster T3-2; Poster T4-7
Morari C	Poster T1-10; Oral T3-5

Movileanu L Pl-7

Mrowczynski R Poster T1-20

Muntean C M Poster T1-2

Muresan-Pop M Poster T1-4; Poster T1-13

Mustafa T Oral T3-3

Nan A Oral T3-2; Oral T3-6; Oral T3-11

Neaga A O Oral T4-3; Poster T4-6

Neamtu C Poster T2-9; Poster T2-10

Negro M Poster T2-11

Nemes P Pl-13

Neumann M Pl-8; Poster T2-8

Nicula C Oral T3-8

Nyari T Poster T3-9; Poster T3-22

Olenic L Oral T3-9; Poster T3-15

Onija O Poster T1-21

Opris O Poster T1-27

Pala M G Pl-6

Pana O Oral T3-7; Poster T3-23

Pasca R D Poster T3-12; Poster T3-13

Pascalau M Poster T3-5

Pascuta P Poster T3-14; Poster T3-24

Perhaia I Poster T1-16

Peter A Oral T3-8

Pirnau A Poster T1-3; Poster T1-9; Poster T1-22

Pogacean F	Oral T3-9; Poster T3-15; Poster T3-17
Pogacian S	Poster T2-6
Pop A V	Poster T3-19
Pop M N	Poster T1-5; Poster T1-6; Poster T1-21; Poster T2-7
Popa A	Oral T1-2; Poster T2-3;Poster T3-16; Poster T3-20; Poster T3-24
Popeneciu G	Oral T2-1; Oral T2-4; Poster T2-2; Poster T3-4
Popescu I C	Poster T3-5
Popescu L B	Oral T3-10
Popovici E J	Poster T3-23
Porras M A	Poster T2-5
Povar I	Poster T1-23; Poster T1-24; Poster T3-7
Pruneanu S	Oral T3-9; Poster T3-15; Poster T3-17
Puscas R	Oral T4-2; Poster T4-9; Poster T4-10
Rada S	Poster T2-3
Radu S	Poster T4-9
Raicu V	Pl-9
Raita O	Oral T1-2; Poster T3-16; Poster T3-19; Poster T3-20
Ratz C	Poster T3-18
Rednic L	Poster T2-8; Oral T3-2; Oral T3-6
Rednic V	Poster T2-8; Oral T3-1
Ristoiu D	Poster T1-32
Rosu M C	Poster T3-2; Poster T3-21; Poster T3-24
Rus L M	Poster T1-25
Santa S	Poster T3-18

Schnadt J	Poster T1-11
Schulte K	Poster T1-11
Scmutzer G	Oral T1-3; Poster T1-19; Poster T1-26; Poster T1-31; Poster T4-4
Sellier H	Pl-6
Shyaka J	Oral T3-3
Silipas T D	Poster T3-2; Poster T3-9; Poster T3-21; Poster T3-22; Poster T3-24
Socaci C	Oral T1-5; Oral T3-2
Socoliuc V	Oral T3-10; Oral T3-12
Song E	Pl-1
Soran M L	Poster T1-14; Poster T1-27; Poster T1-28; Oral T3-7; Poster T3-23
Spangenberg J N	Pl-10
Stagira S	Poster T2-11
Stan M	Poster T1-28; Poster T2-3; Poster T3-20
Stanescu D	Poster T1-22
Stefan M	Oral T3-7; Poster T3-23
Stefan R	Poster T3-16
Steriotis Th	Pl-11
Stoia V	Poster T4-5; Poster T4-11
Suciu R C	Poster T3-2; Poster T3-9; Poster T3-21; Poster T3-22; Poster T3-24
Surducan E	Poster T2-9; Poster T2-10
Surducan V	Poster T2-9; Poster T2-10; Poster T2-12
Susan-Resiga D	Oral T3-12
Szabo I	Oral T2-1
Szelitzky T	Oral T4-3

Taculescu A	Oral T3-2; Oral T3-12
Takeshita K	Pl-12; Oral T4-4
Tapaszto L	Pl-13
Teodorescu C M	Oral T3-7
Tigae C	Poster T1-16
Tiusan C	Pl-14
Toadere F	Oral T2-5
Toloman D	Poster T3-20
Tomoaia-Cotisel M	Poster T3-12; Poster T3-13; Poster T3-18
Tomuta I	Poster T1-25
Tosa N	Poster T1-10; Poster T1-29; Oral T2-5; Oral T2-6
Tosa V	Poster T2-5; Poster T2-11
Tripon C	Poster T1-8; Poster T1-30
Trosan L	Oral T1-1
Trusca R	Oral T2-1
Tudoran C D	Poster T2-12
Turcu I	Oral T1-5; Poster T1-17
Turcu R	Oral T1-5; Oral T3-2; Oral T3-6; Oral T3-11
Turdean G	Poster T3-5
Turrina A	Oral T1-4
Tusa F D	Poster T1-31; Poster T4-4
Tutu H	Oral T3-8
Umwungeri J L	Oral T3-3
Varodi C	Poster T1-28; Poster T3-24; Poster T3-25; Poster T4-5; Poster T4-11

Vekas L Oral T3-2; Oral T3-11; Oral T3-12

Velotta R Poster T2-11

Vida-Simiti I Poster T4-1

Vlassa M Poster T1-31; Poster T3-4

Voica C Poster T1-32; Poster T2-13; Poster T4-10

Vozzi C Poster T2-11

Vulcu A Poster T3-25

Wallart X Pl-6

Wang B Poster T1-11

Watanabe F Oral T3-3; Poster T3-3

Weinmann S Pl-1

Wu Z H Pl-15

Xie Y N Oral T3-13

Yacob Z Poster T2-4

Yan L Pl-1

Zhang J Oral T3-1; Oral T3-13

Zhen L R Oral T3-13

Zotoiu D Poster T2-6