11th International Conference

PROCESSES IN ISOTOPES AND MOLECULES

Cluj-Napoca 2017

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Welcome at PIM 2017

It is a pleasure of the National Institute for Research and Development of Isotopic and Molecular Technologies to host the 11th International Conference Processes in Isotopes and Molecules (PIM).

The PIM conference, which 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.

PIM 2017 provides a unique communication and discussion platform in a wide range of topics, from fundamentals in physics and chemistry, to applied research on energy efficiency, environment, materials and isotopic technologies. Besides the regular scientific sessions, held during the first two days of the conference, the last day will be entirely devoted to bringing together RD&I and industry within the micro-symposia: *Clustering Alternative Energies across Europe*.

The social program will provide participants with an opportunity not only to relax after meetings, but also to experience touristic attractions in Cluj-Napoca and the surroundings.

Topics:

T1 – Stable Isotopes, Labeled Compounds and Analytical Techniques

T2 – Molecules, Biomolecules and Green Technologies

T3 – Energy Efficiency and High-Tech Engineering

T4 – Nanostructured Materials - Nanocomposites and Hybrid Materials

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

Recycling of organic waste as part of circular economy: Solution to prevent environment spreading of contaminants and microbial resistance including application of nano- and microparticles

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Abstract. Recycling of organic waste resources is required in order to develop a circular economy and sustainable living. Organic waste resources can contain heavy metals, organic contaminants, residues of human and veterinary pharmaceuticals, and antimicrobial resistance (AMR) that might represent a risk to the environment or the human health. Organic wastes resources containing xenobiotics, AMR or AMR genes are for instance manure from treated livestock, sewage sludge, fish sludge, organic waste from flower production. Waste management and remediation technologies should be designed and optimized to reduce the content of xenobiotics, AMR or AMR genes in organic waste resources. This presentation will discuss application of nano- and microparticles in environmental technologies focusing at recycling of organic waste.

Plenary Pl-2

Compound-specific isotope analysis to improve food traceability

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Abstract. The scandals of recent years have left their mark on consumer confidence in food products. For this reason there is increasing demand for analytical techniques able to provide data on issues such as the traceability, authenticity and origin of foods and beverages. Stable isotope ratios have been used for food authentication for thirty years, and in the last few years emerging methods aimed at individual chemical compounds have provided a means of obtaining a more in-depth understanding. In particular, a technique that shows enormous promise in this area is gas chromatography combustion/pyrolysis - isotope ratio mass spectrometry (GC-C/Py-IRMS). This technique can be applied to a wide array of foods and beverages, generating data on key food components such as amino acids, fatty acids, aroma compounds and carbon dioxide (in carbonated beverages). This data can be used to verify the geographical origin of foods and food ingredients and the use of synthetic or organic fertilisers, as well as to determine the synthetic or natural origin of food ingredients. GC-C/Py-IRMS is thus one of the most powerful techniques available at the moment to detect fraudulent, illegal, or unsafe practices in the food and beverage industry.

Plenary Pl-3

Rare-Earth Elements in the Environment: Tracers of Natural Biogeochemical Processes vs. Anthropogenic Disturbance of their Distribution

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Abstract. The rare-earth elements (REEs) are comprised of the elements from atomic number 57 (La) to 71 (Lu) and display coherent geochemical behaviour. Their distributions and inter-element relationships in different natural environments have been successfully used as tracers of biogeochemical processes. However, REEs belong to the group of critical elements that are key components for the development of new technologies, such as wind turbines, electrical car engines, medical diagnostics and petroleum refining, and this has led to disturbance of their natural distribution in several aquatic systems. In this presentation both scenarios will be covered: (i) the utility of REEs as effective tracers of the provenance of settling matter in a dated sediment core from the North Atlantic, and (ii) the impact of the emerging technologies on the disturbance of the REEs distribution in the Guadalquivir Rivir (Gulf of Cadiz, South Spain).

Plenary Pl-4

DarkSide-20k and Aria, two massive and technological projects for the Dark Matter research with Ar-40: their broader impact and transfer technology

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Abstract. The DarkSide collaboration, through the operation of the DarkSide-10 and DarkSide-50 detectors, has demonstrated that the two-phase argon Time Projection Chamber (TPC) operated with argon depleted from 39Ar is a viable candidate for this compelling science program. Two years ago, the DarkSide collaboration proposed to Gran Sasso Laboratory (LNGS), DarkSide-20k, designed to reach, in a background-free condition, exposures of 100 tonnexyr. DarkSide-20k will consist of a 30-tonne depleted argon detector with a 20-tonne fiducial mass, to be commissioned and operated at LNGS within 2020. The Aria project was developed within the DarkSide collaboration with the initial purpose of providing means of further depleting the underground argon and consists mainly of a cryogenic distillation plant. It will exploit the fact that different isotopes of the same molecule have a tiny difference in the vapor pressure. If the distillation column has enough equilibrium stages, the separation between isotopes, very similar in mass, becomes possible. The high number of equilibrium stages translates to a very tall column, leading to the Monte Sinni Mine being identified as the ideal place to realize such a project because of the presence of its very deep shafts. The development of the Aria project in the isotopic separation of argon for DarkSide, is also of great interest among other fields. We believe that the technology we are developing will be able to produce other rare, stable isotopes on a large scale, at a competitive cost. At the moment, there are two main fields that have been taken into consideration:

1. The medical field, benefitting from the production of ^{18}O and ^{13}C.

2. IV generation nuclear power plants, interested in the production of ^{15}N.

Plenary Pl-5

Targeting K-Ras for Anti-cancer Drug Discovery

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Abstract. K-Ras is a key molecular switch that controls numerous cell-signaling pathways whose over activation due to mutation is associated with ~25% all human tumors and up to 90% of specific tumor types. Thus a drug that directly and selectively inhibits K-Ras would be a game changer in cancer therapy. However, finding such a drug has remained elusive for a number of reasons. One challenge is that the catalytic site is an unsuitable target because it is conserved in many families of GTPases. Even if selective inhibitors of the active site were identified, the high concentration and affinity of cellular GTP and GDP would make competitive inhibition impractical. Since K-Ras is a small, monomeric protein with a somewhat flat surface, alternative ligand binding sites were not seriously considered. As a result, it was thought that direct inhibition of K-Ras would be impossible and efforts were diverted toward indirect inhibition, such as interference with the membrane binding of K-Ras. Recent advances have allowed for a re-imagination of direct inhibition, and it is now well accepted that K-Ras is an allosteric enzyme with multiple allosteric ligand-binding sites. Building on these developments, we conducted a large-scale high-throughput *in silico* screening campaign against many different ensembles of solution and membrane-bound K-Ras structures and assessed the Ras binding potential and inhibitory activity of the predicted hits by NMR, fluorescence-based assays, and assays in cells expressing oncogenic mutant K-Ras. I will discuss the discovery and characterization of novel compounds that bind to K-Ras and allosterically modulate its activities in cells as well as purified systems.

Plenary Pl-6

Programming electronic and spin states in 2D supramolecular architectures by single atomic or molecular modifications

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Abstract. Future quantum technologies rely on the understanding of the interaction between different electronic states in atoms or molecules. Surface supported atomic and molecular systems provide a base for such investigations with the particular advantage of addressability. Here we establish on-surface architectures which exhibit extraordinary magnetic and quantum properties originating from the reduced dimensionality of the self-assembled and atomically precise architectures. Quantum well arrays, exhibiting band-like electronic states emerge from the interaction of porous on-surface networks with 2D surface states. By designing the Xe filling pattern in the array, a quantum breadboard can be realized in remembrance of the breadboards used for testing electronic circuitry. 2D 'checkerboard' architectures of magnetic molecules containing different e.g. Fe, Mn spins, on the other hand, exhibit surface enabled magnetic phenomena like a 2D ferrimagnet emerging from the Kondo / RKKY interaction.

Plenary Pl-7

Darijo Lazic

Lazić CONSULTING Srbac

Plenary Pl-8

The role of active site flexible loops in catalysis and of zinc in conformational stability of *Bacillus cereus* 569/H/9 β-lactamase

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Abstract. Metallo-β-lactamases catalyse the hydrolysis of most β-lactam antibiotics and hence represent a major clinical concern. The conformational properties of the BcII β-lactamase have been studied in the presence of chemical denaturants, using a variety of techniques, including enzymatic activity measurement and fluorescence, circular dichroism, and 2D NMR spectroscopies. The data from the various experiments provide evidence that binding of two zinc ions not only increases the conformational stability of the BcII metallo-β-lactamase, but also restores the 3D structural organization that is lost for apoBcII unfolding in the presence denaturant. Moreover the results highlight the importance of a relatively well-defined conformation for two loops that border the active site in order to maintain enzymatic activity.

Plenary Pl-9

Implementing nZEB Skills in Romanian High Education Curricula

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Abstract. Through EU programs were developed a series of training schemes for operators involved in nZEB (near Zero Energy Buildings). These energy efficiency, architecture and environmental courses are focused on providing electrical, civil, installation, mechanical engineers, architects and other professionals, a whole range of knowledge around energy efficiency in the home relating to building systems. This paper provides explanations regarding the educational materials used in case of the accredited full-time course organized by the Technical University of Cluj-Napoca, Romania, through Department for Continuous Education, Distance Learning and Part-time Courses.

Plenary Pl-10

Eco-designed Polymers & Industrial Waste Valorization

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Abstract. European strategic sectors require more sustainable materials and need to fulfill **European regulation in terms of circular economy, recyclability and end of life**. Integrated plastic management & strategies are set up to lead to increased recyclability, sorting and high-quality recycling, management of non-packaging plastics, prevention of single-use plastic items, or reduction and remediation of littering. According to the latest market data compiled by European Bioplastics, global production capacity of bioplastics (bio-based and biodegradable polymers) is predicted to quadruple in the medium term, up to approximately 7.8 million tons in 2019. Even if, at present, bio-based plastics are gaining importance in sectors such as packaging and consumer goods, other sectors with high demanding requirements have still a limited use of bio-based materials. For these structural applications biorenewable resources can be used to tailor structures for formulations which can play an important role as functional materials. This presentation focuses on the topics of eco-designed thermosets, starting with their elaboration in the perspective of tuning the final properties. Then, the problematic of valorization of a biorefinery's side stream will be presented. Finally, will be shortly introduced the topics of **100% recyclable materials** & **innovative composite formulations fully recyclable** obtained from **natural resources**. The associated studies are projected to have a direct impact in environmental terms, reduction of oil based resources (sustainability), eco-design (fully recyclable and reusable composites), high efficient processes (energy consumption reduction) and reduction of generated waste (valorization of residues).

Plenary Pl-11

Utilization of waste heat from aluminium melting furnace

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Abstract. Worldwide production of aluminium consumes about 3.5% of the total global electric power. During the aluminium production, 50% of the supplied energy is consumed by the chemical process, and 50% of the supplied energy is lost in form of heat. Heat losses are necessary to maintain a frozen side ledge to protect the side walls, so extra heat has to be wasted. In order to increase the energy efficiency of the process, it is necessary to significantly lower the heat losses dissipated by the furnace's external surface. Goodtech Recovery Technology (GRT) has developed a technology based on the use of heat pipes for utilization energy from the waste heat produced in the electrolytic process. The heat recovery system can control the ledge thickness and thermal energy can be utilized by other energy demanding processes and increase the aluminium production by 20% and still achieve thermal balance. With heat recovery system 10-12% of the total energy consumption for the furnace can be recovered.

Plenary Pl-12

Femtosecond magnetization dynamics in nanostructures

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Abstract. The use of femtosecond magneto-optical techniques allowed during the past twenty years studying the complex processes related to the interaction between light and spins of magnetic materials. In addition to fundamental questions related to the physical processes responsible for the ultrafast demagnetization, controlling the magnetic state of magnetic materials gives access to a broad range of applications. In that context, the knowledge of the magnetization dynamics in structures with reduced dimensionality plays a key role. It can be achieved by combining the high temporal resolution offered by the femtosecond pulses with a high spatial resolution in a confocal microscopy geometry. Here, I will review some of our recent observations related to the dynamics of the magnetization in nanostructures and emphasize the importance of the dynamical magnetic anisotropies in the magnetization precession triggered by laser pulses.

Section T1:

Stable Isotopes, Labeled Compounds and Analytical Techniques

Oral T1-1

Carbon isotopes from peat bog deposits – a proxy for climate and environmental change. A comparative study between two Romanian peat bogs

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Abstract. Peat bogs are important for several reasons: they are one of the major sources of methane in atmosphere, they are the precursor of coal, and they constitute a valuable record of Holocene environmental changes and vegetation dynamics. During the last decade, several studies have demonstrated the potential of stable isotopes ($\delta^{18}O$, $\delta^{13}C$, $\delta^{2}H$, $\delta^{15}N$) in peat bogs as proxies for climatic change, such as temperature, humidity and/or precipitation shifts and to reconstruct Holocene climate at various time scales. In this study, the variation of carbon isotopes with depth in bulk peat material was used to characterize two Romanian peat bogs. The peat cores (6 cm in diameter) were taken for $\delta^{13}C$ analysis from the center of the sites peat bogs with a hand operated Russian sampler. $\delta^{13}C$ values showed a maximum variation of 2.63 ‰ along a 1.03 m long peat core. Variability in the $\delta^{13}C$ of bulk peat profile could be influenced most heavily by the water availably which, in turn, is related to the amount of precipitation at the time.

Oral T1-2

Modelling and simulation of a ^{13}C experimental separation cascade through cryogenic distillation of CO

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Abstract. The paper presents a method for modelling the technological process of the ^{13}C isotope through the cryogenic distillation of CO. The mathematical model is determined applying some specific methods of systems identification, using the experimental data obtained from the separation plant. The obtained mathematical model's validity is tested by comparing the experimental data with data resulted through the proposed mathematical model's simulations. The main advantage involved by an accurate mathematical model is the fact that through its simulation, the appropriate working parameters result, parameters which can be used in order to obtain a certain imposed value of the ^{13}C isotope concentration.

Oral T1-3

Identification for multiple mycotoxins via immunoassay and HPLC-MS/MS in food and feed

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Abstract. To identify multiplexed mycotoxins in food and feed chain, rapid immunoassay and arbitration detection methods were proposed. Series of high specific monoclonal antibody, recombinant antibody, and nanobody against aflatoxin B1 (AFB1), ochratoxin A (OTA), and zearalenone (ZEA), *etc*, were developed. Then, simultaneous detection for multiplexed mycotoxins was studied by using the Au (or Europium, QD)-based lateral flow strip and non-fouling antigen microarray. The limit of detection was lowered to pg/mL. Simultaneous arbitration detection method based on H(U)PLC-MS/MS was also investigated. Either multiplexed immunoaffinity column or solid phase extraction column was used in the sample extraction. Multiplexed mycotoxins (AFB1, B2, G1, G2, OTA, ZEA, and T-2 toxin) were identified by using a multi-immunoaffinity column in a single run.

Poster T1-1

The Calculus of the Operation Parameters at Pressure of the Primary Separation Column of the ^{15}N Production Plant

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Abstract. The relations for calculus of: 10M HNO_3 flow, isotopic transport, ^{15}N molar fraction at the bottom of the separation column, product flow, interphase transfer velocity, height equivalent to the theoretical plate and sulfur dioxide flows in both stages of the product refluxer are presented for ^{15}N separation column with different diameters and 10M HNO_3 feeding flow rates, operated at pressure. In order to produce the isotope ^{15}N at 99 at. % ^{15}N by isotopic exchange in Nitrox system it is desirable to operate the production plant at biggest flow of 10M HNO_3 solution, which allows the ^{15}N production at that concentration on a given plant. That will be possible by operating the plant at pressure as it is shown in this work. At 0.8 atm pressure the isotopic separation at higher flow rates would be practically equal with that obtained at lower flow rates and atmospheric pressure. For constant: HETP = 10.85 cm, ^{15}N molar fraction of the feeding 10M HNO_3, $N_f = 0.00365$, and of the product, $N_p = 0.12$, the variation of the primary separation column product and of the ^{15}N production plant, as a function of the feeding flow with 10M HNO_3 solution, are also presented.

Poster T1-2

Macro- and microelements distribution among *Phaseolus Vulgaris L.* plant parts, irrigated with water having different isotopic composition

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Abstract. This experiment was conducted in order to investigate the accumulation of macro-, micro and toxic elements in various *Phaseolus Vulgaris L.* plant parts (pod, leaf, stem and root) as function of isotopic composition of irrigation water. The purpose of this study was to follow the distribution of macro-, essential and toxic elements in plant parts, in order to exploit the low contaminated soils for plant cultivation. By varying the isotopic composition of used water, the environmental conditions from different geographical areas i.e. tropical areas, temperate areas were stimulated, with the purpose to see the applicability of obtained results in different climatic areas. Also, the absorption and translocation of heavy metals by different plant parts were evaluated. For efficient processing of experimental data set ANOVA, Pearson correlation and Principal Component Analysis (PCA) were employed. In addition, isotopic compositions ($\delta^{2}H$, $\delta^{18}O$, and $\delta^{13}C$) and isotopic enrichment in ^{18}O from plants samples were determined aiming to investigate the influence of different isotopic content of irrigation water on *Phaseolus Vulgaris L.* plant parts.

Poster T1-3

Assessment of polluted areas based on the content of heavy metals in different organs of the grapevine (*Vitis vinifera*)

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Abstract. In this study, the samples of spatial soil and organs of the grapevine (*Vitis vinifera*) were collected from the selected zone near the Mining and Smelting Complex Baia Mare (Northwest Romania). They were analyzed by ICP-MS to determine the content of Cu, Zn, Pb, As, Cd, Ni and Co with the aim of establish if these data may help in the assessment and improvement of the quality of environment in polluted areas such as Baia Mare and its surrounding area. The results obtained from the calculated biological and enrichment factors, as well as from Pearson correlation study confirmed that very useful information is recorded in plant organs: root, stem, leaves and fruit. The results of this study indicated also that the investigated plants species has some highly effective strategies involved in tolerance to the stress induced by heavy metals. In the investigated areas show severe traces of heavy metal pollution with Cu, Zn Pb, Cd wine samples showed concentration below the maximum allowed by the law.

Poster T1-4

Eighteen century Jesus the Savior wooden icon-analytical investigations

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Abstract. The Monarchic (Holy) icon of Jesus Christ portrays Him as Prophet and Teacher, blessing with his right hand, and holding the Holy Scriptures in His left hand. The representation of the Saviour, just like in the case of the Holy Mother, Mary, in the iconographic repertoire of the Monarchic (Holy) icons, is represented in the most personal, unique, singular way, due to the importance of these icons in the church area. It was investigated by several analytical methods both for wooden stand and painting materials. FTIR spectroscopy and DSC analysis were employed for studying the nature and conservation state of the wooden backing. Fir was determined as icon stand and fungal attack of this wood countertop was evidenced by FTIR and DSC methods. FTIR and XRF spectroscopy were used for the investigation of painting materials. Gypsum was used as ground and the following painting materials were used: red-lead and red iron; green- malachite; blue-Prussian blue; for white gypsum and lead white were used. A protein binder was employed. The icon can be considered having the age after 1704, the year of Prussian blue apparition being 1750.

Poster T1-5

The dynamics of dopamine deuteration on the aromatic ring

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Abstract. Dopamine (DA), an amino functionalised derivative of 1,2-dihydroxybenzene, has a major role as neurotransmitter in the nervous system of humans. Due to its properties, DA is responsible for the development of neurological disorders, such as Parkinson's disease, schizophrenia and depression, and used therefore in the medical field as a drug. Since DA can polymerize easily to a widely used polymer (polydopamine) for which the structure is yet unclear, labelling some of the key positions of DA with isotopes will provide insights in polydopamine structure elucidation. In our study, we focused on understanding the dynamics of the deuteration process of dopamine at the positions of the aromatic ring. For monitoring the degree of deuterium incorporation in the molecule during the reaction, liquid NMR technique was used. An increase of the deuteration degree over time could be observed, and at the same time a selectivity of the deuteration process.

Poster T1-6

Use of stable isotopes and chemometric methods as tools for illegal watering detection of wines

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Abstract. This work was focused in providing complementary isotopic data, combined with chemometrics methods as tools for improving the assessment of water addition in wines. For this, an analytical investigation was performed on commercial wines and reference wine samples made in known conditions, along with some wines samples adulterated by controlled addition of water, in terms of their $\delta^{18}O_{water}$ and $\delta^{18}O_{ethanol}$ values correlated with the deuterium distribution (D/H) in ethanol molecule. Measurements of $^{18}O/^{16}O$ and D/H in water and ethanol extracted from wines were performed by continuous flow isotope ratio mass spectrometry (CF-IRMS) and respectively site-specific natural isotope fractionation nuclear magnetic resonance (SNIF-NMR), the obtained data being analyzed by chemometrics methods. In the classification approach two groups of representative samples were used. The first group consist of the authentic wine samples with confirmed/known data on origin and vintage, while the second group is represented by the commercial samples, with declared origin data on the label. Our results describe the isotopic fractionation of stable isotopes H-O during the alcoholic fermentation processes and the importance of using ethanol as internal isotopic reference as practical tool in detecting water addition in wines.

Poster T1-7

Analytical procedures for the determination of some functionalized materials performances used for retention of organic pollutants from waste water treatment plants

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Abstract. Organic pollutants originate from domestic sewage, urban run-off, industrial effluents and agriculture wastewater sewage treatment plants and industry. Waste water with organic pollutants contains large quantities of suspension solids which reduce the light available to photosynthetic organisms and rendering it an unsuitable habitat for many invertebrates. Organic pollutants include different pesticides, fertilizers, hydrocarbons, phenols, plasticizers, detergents, oils and pharmaceuticals. The determination of organic pollutants in water, generally involves the next steps: extraction with organic solvents, clean-up and gas-chromatography separation. For this purpose, an appropriate sample preparation procedure (extraction, enrichment and purification) was developed in order to obtain concentrated extract of target compounds. Moreover, analytical methods including separation, identification and quantification were optimized for the detection of small amounts of compounds from the real samples of water. Also, the performance of the functionalized materials and their ability to remove these pollutants from waste water treatment plants by a selected determination technique (GC-ECD or GC-MS) has been investigated

Poster T1-8

Infant food supplements quality evaluation through complex analytical methods

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Abstract. There is a growing interest by both consumers and industry for the development of food products with functional properties or health benefits. These food supplements are especially important for infants under development, thus their safety status must be unquestionable. However, the use of different raw materials, process, technologies and storage conditions could impact in an undesirable way the food quality and safety status. The purpose of this work was to investigate commercially available infant food supplements targeting: 1) the content of macro/micro nutrients and toxic metals; 2) volatile organic compounds presence that contribute to flavour and aroma composition of food; 3) content of fatty acids and 4) $\delta^{13}C$ to determine the origin of the raw material for these products. These investigations were performed in order to evaluate the quality referred at nutraceutical value and safety status of food supplements.

Poster T1-9

Phytoremediation of hexachlorocyclohexan (HCH) polluted soils using different wild plants

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Abstract. Phytoremediation represents a new alternative to conventional soil treatments, having many advantages such as low cost, in situ remediation or many interactions between plants and contaminants. Lindane (γ-HCH) was a widely used agricultural insecticide until 2009, when Stockholm Convention banned its production and use of this compound and put it on Persistent Organic Pollutants List. This work presents a laboratory study, carried out in order to determine the capability of six different wild plant species to remediate HCH contaminated soils. The plant seeds were placed in soil having three different levels of HCH concentrations. All plants species proved the capability of removal of HCH isomers from soil in different proportions. Generally, the most abundant isomer analysed in plants samples was α-HCH, followed by β-HCH and last, lindane and δ-HCH. Also, an evaluation among different plant parts was fallowed, but no significant differences and tendencies were noticed.

Poster T1-10

Removal of organic pollutants from aqueous solution by adsorption on metal organic framework and graphene oxide based materials

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Abstract. Environmental pollution with hazardous substances is one of the most serious problems worldwide due to its ecological and human health implication. Numerous endocrine disrupting compounds (EDCs) and pharmaceutical products (PP) contaminants have been discovered in various surface, ground and wastewaters, some of which being linked to ecological impacts, even at trace concentrations. In this study three MOFs (UiO-66, MIL-101 and HKUST-1) and two carbonaceous materials were tested in order to assess their effectiveness in eliminating of two organic pollutants Bisphenol A (BPA) and Carbamazepine (CBZ) from aqueous solution, being the first study in this direction. For this, various adsorption parameters were investigated i. e. contact time, initial concentration of pollutants, in order to determine the optimum adsorption parameters. According to Langmuir model, the maximum adsorption capacity (q_{max}) of partially reduced graphene oxide (PRGrO) for BPA and CBZ (346.07 mg/g and 55.13 mg/g respectively) is higher than q_{max} of graphene oxide (GO) (92.40 mg/g and 32.35 mg/g respectively). Therefore, PRGrO is the ideal adsorbent, for both BPA and CBZ.

Poster T1-11

Determination of capsaicinoids for vegetable oil adulteration by immunoaffinity chromatography cleanup coupled with LC-MS/MS

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Abstract. Capsaicinoids were selected as adulteration markers to authenticate vegetable oils. In this study, a method of immunoaffinity chromatography (IAC) combined with LC-MS/MS was established for the determination of capsaicin and dihydrocapsaicin in oils. In this method, the major parameters affecting IAC extraction efficiency, including loading, washing and eluting conditions, were also investigated. The LODs and LOQs for capsaicin were 0.02 and 0.08 μg kg^{-1}, and for dihydrocapsaicin were 0.03 and 0.10 μg kg^{-1}. The recoveries of in oils were in the range of 87.3%-95.2% with RSDs of less than 6.1%. The results indicated that capsaicinoids could not be found in edible oils. Therefore, the proposed method is simple, reliable and adequate for routine monitoring of capsaicinoid compounds in vegetable oils and has an excellent potential for detection of adulteration with inedible waste oil.

Poster T1-12

Survey on the authenticity of the cider commercialized on Romanian market

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Abstract. Cider is, by definition, a beverage obtained through the fermentation of apple or pear juice. In order to assess the authenticity of the cider that is commercialized on Romanian market, 32 bottled and canned ciders samples were analyzed by mean of stable isotope ratios and elemental profile. Determination of $\delta^{18}O$ values of water from ciders is today an applied and acknowledged method for the detection of exogenous water while, the determination of δ ^{13}C from ethanol and dry substance is a good probe for detecting the addition of cane sugar or maize glucose syrup. Based on the different photosynthetic metabolism of CO_2 plants are spitted in three categories: C_3 (most of the plants including beet sugar), C_4 (e.g. sugar cane, corn) and CAM (e.g. pineapple, cactus); each of these categories being characterized by different rages of variations of $\delta^{13}C$ values. By, using these approaches, the detection of exogenous water and sugars was made for all investigated samples. Beside this, investigation on the differences that occur, in terms of elemental profile, among the bottled and canned cider was performed.

Poster T1-13

Sorption reactions at the two ends of uranium band in ^{235}U isotope enrichment column

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Abstract. In the case of ^{235}U isotope enrichment by chemical exchange in $U(VI)_{(R)} - U(IV)_{(S)}$ system in a column filled with Dowex-Marathon anionic resin, for uranium band displacement, Ti(III)/HCl is used as reduction agent and Fe(III)/HCl as oxidant agent. In the rear boundary of uranium band, $U(VI)_{(R)}$ is reduced to $U(IV)_{(S)}$ and in the front of the uranium band, $U(IV)_{(S)}$ is oxidated to U(VI), which is readsorbed on anionit. In this work, UVI)/HCl and Fe(III)/HCl sorption kinetics on Dowex-Marathon resin were studied. The processes are well described by the pseudo-second order kinetic model for 0.02-0.1 M U(VI)/HCl and 0.05-0.15 M Fe(III)/HCl concentrations. The activation energy for U(VI) sorption is $E_a = 6.62 \pm 0.16$ kJ/mol and for Fe(III) sorption is $E_a = 7.96 \pm 0.2$ kJ/mol, indicating a physisorption process in both cases. It was demonstrated that Dowex-Marathon resin is not suitable for ^{235}U enrichment process by chemical exchange because it presents a low sorption/desorption rate.

Poster T1-14

Wastewater decontamination using low-cost adsorbent materials obtained from agricultural waste

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Abstract. Agricultural biochars obtained from pyrolysis of corn cob, pistachio husk, nut shells, peanut shells, and wood ash, were characterized for their properties and sorption behaviour of organic pollutants from triazines and phenylurea herbicides classes (ametryn, prometon and monuron) and trace amounts of some metals. The pyrolysis of studied materials was made at different temperatures (400 °C, 500 °C and 600 °C) in different conditions: in the presence of oxygen and under argon atmosphere. For the separation and quantification of organic compounds, High Performance Liquid Chromatography with diode array UV detection (HPLC–DAD-UV) was used, and the analytical technique for trace metals measurements was Inductively Coupled Plasma Mass Spectrometry (ICP-MS). The removal rate of different organic compounds and toxic metals pollutants were calculated.

Poster T1-15

Silver wound dressings: comparison of the antimicrobial efficacy of commercially available dressings

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Abstract. The silver antimicrobial dressings have been extensively used as therapeutic strategies in wound management. The present study sought to asses and compare the antimicrobial efficacy of commercially available modern silver wound dressings. The antimicrobial activity of the silver dressings has been evaluated by the disk diffusion method, including four common wound pathogens. The silver release profile has been determined by using Inductively Coupled Plasma Mass Spectrometry (ICPMS). The results demonstrated different degrees of efficacy against the tested pathogens, but we could not establish a correlation between the silver content/silver-release profile and the antimicrobial activity of the evaluated dressings. Different factors such as the structural properties of support-materials, or the form of silver contained may influence the effectiveness of silver dressings. This suggests that silver containing dressings act by a combination of antimicrobial activity and fluid handling properties. Therefore, dressing selection must be decided on an assessment of the overall characteristics of the dressings involved.

Poster T1-16

Appearance of water micropollutants in water as effects of extreme meteorological events

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Abstract. The quantity of anthropogenic compounds released into environment and their potential adverse effects to environmental and human health represent major challenges in the scientific community. For that reason, developments in instrumentation and methods are increasing towards the study the structure and quantity of the compounds present in environmental matrices. In respect to this, one of priorities is to determine the environmental distribution of organic pollutants in the surface waters. The objective of the present study is to obtain data on micropollutants sources present in surface and drinking water after extreme meteorological events in Romanian regions. The analyses were performed on water samples collected from potable water sources using GC/MS method after LL extraction. Were detected and discussed anthropogenic compounds from following compound groups: lubricant and plastic additives and hydrocarbons. The compound identification was done based on mass spectra obtained by Electron Impact ionisation in full scan mode.

Poster T1-17

Stable isotopes determination in edible mushrooms from the spontaneous flora of Transylvania

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Abstract. The edible mushrooms represent a food product highly appreciated in the culinary art. In this study, 12 species of edible mushrooms from the spontaneous flora of Transylvania, summing 89 samples, were investigated from stable isotopes point of view ($^{2}H/^{1}H$, $^{18}O/^{16}O$ and $^{13}C/^{12}C$) in order to isotopic fingerprinting these plants. The sampling period was 2015-2016. The isotopic values of samples ranged between -68.3 ‰ and -7.6 ‰ for deuterium, and between -9.1 ‰ and 1.7 ‰ for oxygen-18, respectively, reflecting the geographical origins of studied mushrooms. The obtained results ($^{2}H/^{1}H$, $^{18}O/^{16}O$) were in good correlation with the meteoric water line for the Transylvania region. Beside this, using the isotopic fingerprint of mushrooms from the Transylvania spontaneous flora it could be distinguishing the growing location of different samples: a hilly area (with an altitude up to 500 m) and a mountainous area (with an altitude between 500 m and 1000 m).

Poster T1-18

Chemometric approach for the differentiation of greenhouse grown vegetables from those cultivated in the field

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Abstract. Traceability of vegetables represents nowadays an important issue for consumer's perception. In this regard, the differentiation markers that could distinguish greenhouse vegetables from those produced in the field were investigated in this study. In order to asses this goal, the isotopic and elemental profile was determinated for two lettuce sorts (Murai and Redial) grown both in the greenhouse and on the field. The growing period was about 3 months while samples were taken weekly. By applying LDA (Linear Discriminant Analysis) a differentiation between the two grown lettuces types (greenhouse vs. field) was made in a percent of 81.8 % for initial classification whereas for cross-validation the obtained percent was 77.3. The best predictors for this classification have proved to be: Li, Ba and Cu. For the differentiation between the lettuce sorts (Murai and Redial), the same statistical approach was used and for this purpose, the best identified marker was $\delta^{13}C$. In this case, the initial and cross-validation classification was 70.5 %.

Poster T1-19

Improving semiquantitative analysis for water samples, using a fast multielement spectrometric method

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Abstract. Semiquantitative spectrometric methods offer a fast overview for elemental concentration in a sample, but it's not always an accurate method for every measured element. Improving the algorithms for data interpolation used in building the response factor and using the appropriate calibration could improve method accuracy without compromising the time required for analysis. Water samples from Someș, Prut and Bîc rivers were analyzed over the course of two seasons using three spectrometric techniques in two laboratories (ICIA and UnAȘM) and the obtained results were used to improve semiquantitative method. Cr, Mn and Cu concentrations were within accepted accuracy interval, Pb was below detection limit and semiquantitative method failed initially to provide a result within expected accuracy for Zn and Ni. Method improvements lead to better accuracy for results and to an extended array of analyzed elements.

Poster T1-20

Optimization of polyphenols extraction from hawthorn fruits

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Abstract. The forest fruits are an important source of bioactive compounds with various application in medicine and food industry and due to this, an important goal is to find the optimum extraction method. The aim of this work was to obtain the extracts from hawthorn fruits with the highest content in polyphenols. The optimization was performed using Minitab 17 software and Box-Behnken design, introducing time, temperature and solvents ratio as variables. The sonication and reflux were tested as extraction techniques. The best extracts were obtained by sonication for 10 minutes at 80°C with 55% food ethyl alcohol, when the total content of polyphenols was 3.02 g gallic acid / 100 g dried plant. These extracts were used for sweets preparation instead of chemically aroma.

Poster T1-21

Removal of Toxic Metals from Water Using Nanostructured Carbon Materials

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Abstract. Contamination of water by toxic heavy metals through the discharge of industrial wastewater is a worldwide environmental problem. The adsorption from aqueous solution of trace amounts of some metals using nanostructured carbon materials (ordered carbon, graphene oxide and partially reduced graphene oxide), as highly adsorbent material, has been studied through batch experiments. The choice of these materials was made based on their very particular properties: high surface area, controlled porosity, the possibility to tailor the surface hydrophilicity. The materials characterization sought to determine some important parameters for adsorption properties such as: (i) surface area and porosity, (ii) surface properties: acidity, degree of oxygenation, (iii) crystalinity, (iv) moisture and temperature stability. The trace metals determinations were performed by an Inductively Coupled Plasma Mass Spectrometer (ICP-MS), Elan DRC-e Perkin Elmer. For each sample analysis three replicates were measured in order to assure the control quality.

Poster T1-22

Aflatoxin contamination of peanuts at harvest in China and its relationship with climatic conditions

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Abstract. Aflatoxins are toxic, mutagenic, and carcinogenic compounds and contaminate various agro-products, especially peanuts. A total of 2494 peanuts from four major peanut producing areas in China from 2010 to 2013 were investigated for aflatoxins occurrence. A close relationship was concluded between the result and the weather a month before harvest. The highest aflatoxin contamination level occurred under the climatic conditions where precipitation was rare and the mean temperature was close to 23°C. The minimum and maximum temperature for the occurrence of aflatoxin was approximately 20°C and 29°C, respectively. It provided valuable information on aflatoxin contamination in pre-harvest peanuts under different agro-environmental conditions in China and laid a foundation for predicting aflatoxin contamination, which would be essential for taking preventive measures to alleviate pre-harvest aflatoxin contamination of peanuts.

Poster T1-23

Authentication of edible vegetable oil based on fatty acid profiles and chemometric methods

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Abstract. Edible oils are the most frequently counterfeited food. The more effective adulteration detection model should be built to quality inspection of edible oil in practice. The aim of this study was to develop a robust model for authentication identification of edible oils and determine the lowest detectable adulteration level (LDAL). Random Forests (RF) and one-class partial least squares were combined to identify the authenticity of edible oils by fatty acid profiles. Classification model was built by RF for five kinds of edible oils. Subsequently, the OCPLS model was established. The validation results that the RF could identify the all kinds of edible oils and OCPLS classifier could completely detect the adulterated oils and are therefore employed to authenticity assessment. As an example, the LDAL of OCPLS model was determined as 8% for rapeseed oil. The built model is helpful in quality inspection of high-price edible oil for protecting the customers far from adulterated edible oil.

Section T2:

Molecules, Biomolecules and Green Technologies

Oral T2-1

In vivo ^{1}H NMR spectroscopy and relaxometry maps of woman's pelvis

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Abstract. Essential organ of the female reproductive system, the uterus is divided, histologically, in three layers: the perimetrium, the myometrium and the endometrium. *In vivo* NMR imaging, spectroscopy or relaxometry are modern NMR methods that becomes important tolls used by radiologist to increase the degree of confidence in their diagnostic, in particular to provide noninvasively metabolic information and establish a standardized characterization of the nonpathological tissue. We propose a series of MRS examination correlated with the T_1, T_2 and ^{1}H spin density maps in order to establish the average values and variation of relevant NMR and bio-chemical parameters on non-pathological woman's pelvis endometer. This study assumes: i) a series of data analysis steps performed by jMRUI^{TM} software are used for data import and primary NMR signal processing (water and metabolite signal separation, phase and baseline correction, apodization for noise reduction, LPSVD quantification for fat signal extraction from ^{1}H NMR spectra) and ii) an advanced analysis based on dedicated programs written in Processing^{TM} software. Finally, relaxation times values and metabolites' characteristics are statistically correlated.

Oral T2-2

Mapping, characterization and specific inhibition of allosteric protein-protein interactions in signalling networks involved in tumorigenesis and inflammation

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Abstract. Cancer and inflammation are related disorders. These pathological phenomena arise as consequences of disturbances in certain cellular signaling networks. Revealing and describing the underlying protein-protein interactions in these networks is the way of understanding these signaling pathways. These pathways are organized into networks. In case of disturbances in certain signaling pathways, intervention must be specific to the abnormal process and should not affect the normal function of the organism (side effects). The means to achieve this is to target the specific allosteric protein-protein interactions. Rassf1A is a major tumor suppressor regulating cell cycle by mitotic arrest. Down regulation of Rassf1A by specific phosphorylation by Aurora A kinase results in unregulated mitotic progression. To map the recognition signal of Aurora A on Rassf1A we designed both a pseudo-activation loop and a domain deletion mutant of Rassf1A. We showed that both parts are essential for the specific recognition and phosphorylation of Ser-203 of Rassf1A by Aurora A. ROCK2 kinase phosphorylates both Amyloid Precursor Protein (APP) and β-secretase (BACE1) on their intracellular flanking regions. Specific inhibition of this phosphorylation event reduces the formation of Aβ40 and Aβ42, both relevant peptides in Alzheimer disease. We developed a screening cascade to find pathway specific inhibitors for the ROCK2 versus APP or BACE interaction. We have revealed that an allosteric binding site exists for the APP-ROCK2 interaction.

Poster T2-1

Assessment of metals content in dandelion (*Taraxacum officinale*) leaves grown on mine tailings

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Abstract. Dandelion (*Taraxacum officinale*) is one of the plant species that has the ability to spontaneously grow on mine tailings, due to its high tolerance for harsh environmental conditions (low nutrients level, high metal contents). The concentrations of Cd, Cu, Pb and Zn were determined in tailings and dandelion leafs grown on nonferrous mine tailings from Romania, while the metal accumulation was assessed by transfer factors (TFs) calculated as the ratio between the metal concentration in plant leaves and in tailings underneath. The results showed that metal concentrations in tailings ranged between 0.4-8.0 mg/kg Cd, 20-1300 mg/kg Cu, 27-570 mg/kg Pb and 48-800 mg/kg Zn, while metal concentrations in dandelion ranged between 0.2-4.8 mg/kg Cd, 6.2-17 mg/kg Cu, 0.5-75 mg/kg Pb and 27-260 mg/kg Zn. The TFs were below 0.8 for Cd and Zn and below 0.4 Cu and P and decreased in the following order Cd≥Zn>Cu≥Pb, suggesting the Cd and Zn accumulation capability of dandelion.

Poster T2-2

Low-lying excited states and their relaxation pathways of phenothiazine

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Abstract. The first two, low-lying electronic excited states and their relaxation pathways for the phenothiazine has been investigated using multi-configuration self-consistent field, equation-of-motion coupled cluster and density functional theory (DFT) methods considering the def2-TZVP triple-ξ quality basis set as well as the MN12-SX exchange correlation functional in the case of DFT. The electronic configurations of the first three vertical excited states as well as the geometries of conical intersections between different excited states were discussed in details. Different relaxation pathways over the potential energy surfaces are identified and discussed.

Poster T2-3

Advanced methods for the characterization of commercial cosmetics effects on the skin

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Abstract. The skin diseases are one of the contemporary important social topics. It is a general behaviour of people from modern society to cover the skin defects by applying a thin layer of cosmetic emulsions, gels, etc. One-dimensional (1D) and two-dimensional (2D) Nuclear Magnetic Resonance relaxometry correlated with advance data processing by the 1D and 2D Laplace inversions methods are advanced methods used in the study of such type of commercial cosmetic materials. We investigate tree types of body creams and their action upon natural and artificial skin. In particular, the test samples are sheets of three layers of 1 mm silicon rubber glued with New Skin liquid bandage thin film on natural deer leather. The microscopic properties are obtained from a series of i) NMR methods (CPMG, Hahn-echo and T_1-T_2 correlation maps and self-diffusion) ii) hydration/dehydration processes were monitored by electric conductibility local measurements using a dedicated sensor inserted between silicon rubber and deer leather. The creams were subject to UV radiation with increased time period and the microscopic properties were measured again and statistically analysed. We found that even at five minute the UV radiation changes the dynamic properties of body creams cosmetics.

Poster T2-4

Tracking some emerging environmental contaminants acting as endocrine disruptors

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Abstract. A wide variety of emerging environmental contaminants affect the endocrine system, being called endocrine disruptors. Among them are encountered the organochlorine pesticides (OCPs) and polychlorinated biphenyls (PCBs), generically grouped under the name of organochlorine compounds (OCs). Their assessing in environmental samples requires selection of very sensitive analytical methods, since these compounds are present in the sample in low concentrations and consequently the detection level imposed by the legislation is very low. In our work, a gas-chromatographic method coupled with Electron capture detector (GC-ECD) was used. The samples were taken from different local breeders, from Valcea, the investigation being performed on soil and water samples and progressing to vegetation and milk. The predominant compounds being the HCH and DDT. PCBs were detected in all the analyzed soil samples, registering for the individual compounds values lower than the alert levels set by national legislation (Order 756/1997) for sensitive soils, with the exception of concentration for the PCB28 compound in 4 soil samples, namely 8.01 µg/kg in sample 3, 5.02 µg/kg in sample 4, 6.72 µg/kg in sample 5 and 3.09 µg/kg in sample 2. Efforts should be focussed in further tracking of these contaminants and on the evaluation of their effects on human health.

Poster T2-5

Rapid, accurate, and comparative discrimination of clinically relevant fungi via SERS fingerprinting and robust chemometric techniques

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Abstract. Candidiasis and aspergillosis are the most often fungal infections (FI) found in clinical practice, especially in immunocompromised patients. Classical methods of FI diagnosis - blood testing, or culturing, can take from days to weeks. An alternative analysis and diagnosis tool is embodied in the surface-enhanced Raman scattering (SERS) combined with powerful chemometrics. Thus, the whole-cell fingerprint SERS spectra, recorded by using an innovative *in situ* approach were thoroughly analysed by using Principle Component Analysis (PCA). A reliable, fast and high-accuracy discrimination between pathogens with similar spectral profiles was achieved.

Poster T2-6

Structure – biological activity profile of *Plantago* flavonoids with estrogenic potential

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Abstract. Flavonoids are a group of secondary metabolites found in plants, in a high concentration especially in *Plantago* species. Known for their antioxidant properites, this class of compounds are structurally similar to estradiol. Based on this hypothesis, a new strategy for antioxidant and hormonal replacement therapy could be found. Our study aims to investigate the positive interactions between estrogenic flavonoids and estrogen receptors, alpha and beta. Activation of estrogen receptors, mostly beta (ER-β) is an essential mechanism for the prevention of many diseases. Using computational methods, such as Molecular Docking, we could predict the orientation of the molecules of interest, such as luteolin, apigenin and rutin. Aditionally, the formation of molecular complexes could be investigated, by their geometric affinities of bonding and association parameters.

Poster T2-7

Multiscale models of wild-type and G12V mutant Nras oncogenic systems

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Abstract. Ras oncoproteins belong to a class of GTPase switch proteins that have an essential role in activating signaling pathways responsible for growth, proliferation and differentiation. Mutations in different Ras isoforms, Hras, Nras and Kras, have been implicated in the pathogenesis of different cancers. The most common mutation in Nras occurs at positions 12 (G12) and affect the normal cycle between GDP-bound inactive and GTP-bound active states. So far, no successful effective therapeutic approaches to directly target mutant Ras have been identified. Hence, we propose a multiscale *in silico* modeling of the Ras oncogenic systems. First, we used atomistic models to study NRas (both wild-type and mutant G12V) protein's interaction with the cellular membrane. However, since NRas proteins assemble into transient, nano-sized substructures, difficult to access by atomistic simulations or experimental techniques, we employed semi-atomistic coarse-grained models to study their association mechanisms. We combined molecular dynamics and docking simulations to characterize the system dynamics and identify binding sites of novel potential drugs, respectively.

Poster T2-8

The bactericidal activity of some penicillins revealed by electronic structure and molecular docking

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Abstract. Penicillins are a group of natural antibacterials, part of β-lactam antibiotics class, semisynthetisized from *Penicillium* mould. One "spokesman" for each of the five generations – benzylpenicillin (BPN – 1st generation), oxacillin (OXN – 2nd generation), ampicillin (APN – 3rd generation), carbenicillin (CBN – 4th generation), and azlocillin (AZN - 5th generation) – was chosen to be investigated. Taking into account their action on Gram-positive, Gram-negative or both, we focus on the way in which the structural differences of the side chains attached to the common penam core (a 6-aminopenicillanic acid (6-APA)) influence their bactericidal activity. Several theoretical tools are used. Electronic structures are depicted by molecular electrostatic potentials (MEPs), (re)distribution of electron densities (EDs), and natural bond orbital (NBO) analyses. DFT and molecular docking methods were used to find the connection between the chemical structures and biological activity, on molecules in aqueous media. HOMO, LUMO and HOMO-LUMO gap energies are calculated by TD-DFT to describe chemical reactivity of the molecules. A comparison between the theoretical and experimental electronic UV-Vis spectra is also reported.

Poster T2-9

Crystal engineering in pharmaceutical research

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Abstract. Rivaroxaban (5-Chloro-N-((5S)-2-oxo-3-[4-(3-ox-omorphdin-4-yl) phenyl]-1,3-oxazol idin-5-yl} methyl) thiophene-2-carboxamide), marketed under the trade name Xarelto, is a low molecular weight, orally administrable anticoagulant drug. It is a serine protease factor Xa inhibitor and can be use for prevention or treatment of the thromboembolic diseases. Although Rivaroxaban exist in several polymorphic forms: polymorphs (I, II, III), hydrates (mono-, di-), solvate with N-methylpyrrolidone, co-crystal with malonic acid, clathrate with THF and amorphous form, the crystalline structure is not known for any of these forms. Crystalline structure of the active pharmaceutically molecules has a close relationship with their physical-chemical properties, such as dissolution rate, solubility and stability. All these properties influence their processing and formulation, being very important for pharmaceutical industry. The single crystals of Rivaroxaban in polymorphic form I was prepared by high throughput crystallization process from nitromethane. The crystal structure - namely crystallographic system, unit cell parameters, space group and the atomic positions in the unit cell - were determined by single crystal X-ray diffraction.

Poster T2-10

Molecular interaction between drugs with antimicrobial activity and macromolecular receptors

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Abstract. Antibiotics have improved public health but very success of these drugs has often resulted in an inappropriate and irrational use of antimicrobial drugs. Increasing the number of pathogens resistant to different classes of antibiotics and infectious diseases led to the need to develop a new approach to antimicrobial therapy. With the view to counteract the increasing prevalence of this phenomenon, a large number of research studies have been focused on the development of new molecules with antibacterial and/or fungicidal properties. New quaternary ammonium compounds, having at the basis the 2-aryl-thiazole system diversely substituted at the 2, 4, and 5 positions, have been synthesized. The main goal of our contribution is to provide a complete thermodynamic profile of the binding, in liquid and solid state, of drugs with antimicrobial activity to macromolecular receptors by ITC calorimetry, ^{1}H NMR and XRPD methods.

Poster T2-11

Design of experiments for methylene blue removal on activated carbon using Taguchi methodology

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Abstract. The optimization of various batch parameters (initial dye concentration, adsorbent quantity, contact time, particles size and stirring rate) for the removal of methylene blue (MB) from aqueous solutions using commercial activated carbon (AC) was studied. The experimental data were processed with "larger-the-better" quality characteristics. ANOVA analysis showed that the most significant parameters for MB biosorption onto AC are: initial dye concentration, adsorbent quantity, particles size and stirring rate (small p-values obtained). The experimental data were analyzed using Langmuir and Freundlich isotherm models. Also, Temkin and Dubinin-Radushkevich isotherm models have been considered in order to identify the type of adsorption for the considered process. The preliminary results, indicated that commercial activated carbon is an efficient adsorbent for MB removal from wastewaters.

Poster T2-12

Structural and mechanistic characterization of a new ubiquitin ligase–PRT1 from *Arabidopsis thaliana*

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Abstract. Nowadays, increasing attention is being paid to small molecules involvement in protein metabolism. One such moiety is ubiquitin, a small protein that targets polypeptidic systems for degradation. Its attachment consists of a set of three reactions: activation of ubiquitin via ATP-dependent E1, transportation of the red flag assisted by E2 and the binding to the substrate mediated by E3 ligase. Our research work is based on ubiquitination corresponding enzymes from experimental plant *Arabidopsis thaliana*: UBA1 (E1), UBC8 (E2) and PRT1 (E3). The structures and mechanisms of the first two mentioned enzymes are known, whereas less was unveiled about the E3 ligase, beside the sequence of aminoacids and an observed specificity for aromatic N-terminal residues. The aim of our research was to prove that E3 (a three zinc RINGs containing enzyme) has indeed a discriminatory character toward bulky aromatic aminoacids in the N-end position using western blotting technique. A brief spectroscopic characterization was performed which led us to the scheme of replacing the zinc ions from wild-type PRT1 with transitional metal ions with similar chemical properties and to assay the obtained biomolecules activities toward ubiquitination. Interesting conclusions were drawn which laid the foundation for future research ideas.

Poster T2-13

Vibrational relaxation of LacDNA complexes by UV resonance Raman spectroscopy

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Abstract. Vibrational bandshape analysis through time correlation function concept is widely used to obtain experimental information on the molecular dynamics of small and medium size molecules in different environments. Interesting details are revealed by extending this technique to biomolecules such as functional groups of the nucleic acids in media approaching the physiological conditions. In this work a study into the UV resonance Raman (UVRR) vibrational dynamic parameters of functional groups in LacDNA, upon lowering the pH and in the presence of divalent metal ions, was of interest. The 793 cm^{-1} UVRR band, corresponding to ν (backbone O-P-O, dT) oscillator of LacDNA in aqueous solutions was selected for band shape analysis. Efficient vibrational relaxation of this mode is accomplished by vibrational dephasing.

Poster T2-14

Growth of common bean (Phaseolus vulgaris L.) exposed to electrosmog in a controlled environment

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Abstract. In order to evaluate the effects of electrosmog on crop growth of a common bean (Phaseolus vulgaris L.) cultivar, an indoor experiment was conducted during 2016-2017. The climbing bean was grown in pots with 45 l of soil, on metallic poles acting as antennas, under controlled conditions (watering, temperature and hours of artificial light per day). The irradiated plants were exposed continuously to low intensity 915 MHz (GSM-I frequency) electromagnetic radiation, corresponding to environmental irradiation levels measured for moderately used GSM networks (10 mW m^{-2}). Both control and irradiated plants were measured to determine the total stem length and number of inflorescences per pole, to assess growth at various developmental stages: initial vegetative growth, first flower flush, full flowering. Results indicated that the exposure to microwave radiation increased the stem length and reduced the number of inflorescences of the plants.

Poster T2-15

Interaction of allicin with human serum albumin investigated by fluorescence spectroscopy

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Abstract. Allicin is an organosuphurous compound belonging to the most important class of bioactive compounds in *Allium*, with a high therapeutic potential: antioxidant, antifungal, antimicrobial and antiproliferative. We used in this study the fluorescence quenching method to determine the binding mode, binding parameters and conformational changes that characterize the interaction of allicin with human serum albumin (HSA), the main blood plasma carrier of drugs. Fluorescence quenching of HSA's internal fluorophore (tryptophan, Trp 24) and bi-molecular quenching rate constant of k_q = 2.28 10^{13} $M^{-1}s^{-1}$ calculated from Stern-Volmer equation indicate allicin-HSA interaction with molecular complex formation. It also suggests the affinity of allicin to IIA domain of HSA molecule where Trp24 is located. Synchronous fluorescence data shows no changes in the microenvironment around the Trp residues and therefore no conformational changes of HSA molecule in the presence of allicin. The association constant of the HSA-allicin complex, K_a = 0.887 10^2 M^{-1}, calculated with the adequate equation for 1:1 molecular stoichiometry, indicates a very weak interaction between allicin and HSA. These results suggest that HSA is not the main carrier for allicin. The allicin prefer the unbound state, having thus a larger biodisponibility.

Poster T2-16

Quantitative analysis of zidovudine – HSA interaction based on ITC calorimetry, fluorescence quencing and NMR relaxometry

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Abstract. A quantitative analysis of the interaction between zidovudine (azidothymidine -AZT) and human serum albumin (HSA) was achieved using Isothermal titration calorimetry (ITC) in combination with fluorescence spectroscopy and ^{1}H NMR spin-lattice selective relaxation. ITC directly measure the heat during a biomolecular binding event and gave us thermodynamic parameters and the characteristic association constant. By fluorescence quenching, the binding parameters of AZT-HSA interaction was determined and location to binding site I of HSA was confirmed. Via T_1 NMR selective relaxation time measurements the drug-protein binding extent was evaluated as dissociation constants K_D and affinity index. The involvement of azido moiety of zidovudine in molecular complex formation was put in evidence. All three methods indicated a very weak binding interaction. The thermodynamic signature indicates that at least hydrophobic and electrostatic type interactions played a main role in the binding process.

Poster T2-17

Crystal and molecular structure of a Pitofenone Hydrochloride polymorph

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Abstract. Both Pitofenone and Pitofenone Hydrochloride are antispasmotic drugs which relieves pain and spasms of smooth muscles. Single crystals of Pitofenone Hydrochloride were obtained by slow evaporation from ethanol solution. A suitable single crystal of $C_{22}H_{26}ClNO_4$ Pitofenone Hydrochloride was analyzed and the data have been collected on a SuperNova diffractometer using Cu microsource and an Eos CCD detector. The crystal was kept at 293 K during data collection. The crystalline structure was solved using Olex2, with the ShelXS structure solution program and refined with ShelXL refinement package by least Squares minimization. The Pitofenone Hydrochloride compound crystallize in the $P2_12_12_1$ space group (Z=4) of the orthorhombic crystal system, having the following lattice parameters: a=7,1044(3)Å, b=10,1174(5) Å, c=28,8854(16) Å, $\alpha = \beta = \gamma = 90^o$ and V=2076,23 Å^3. Bond lengths, angle measurements and torsion angles were calculated as well. Hirshfeld surface was computed using Crystal Explorer software in order to get a better understanding how intermolecular interactions take place.

Poster T2-18

Structural features induced in pathogenic bacteria by their interaction with natural and synthetic antibiotic agents

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Abstract. The description of the main structural alterations generated by the interaction between pathogenic bacteria and antibiotic agents, either standard antibiotics or volatile plant derived oils, is an essential topic in understanding the drug action mechanisms at molecular level. To investigate this effect, an original approach based on scanning electron microscopy (SEM) and ultra-sensitive vibrational surface-enhanced Raman spectroscopy (SERS) is employed. Single-bacteria SERS spectra, recorded in the 600-1800 cm^{-1} wavenumbers interval are reported here, for two bacterial strains, namely *Enterococcus durans* and *Aeromonas media*. Spectra-structure correlations for all types of localized vibrations, including bands assigned to proteins, saturated lipids, glycosidic linkages and nitrogenous bases are also discussed. SEM images revealed that the mechanism of action of antibiotic agents against the pathogenic microorganisms is a complete denaturation of bacterial membrane, which induces apoptosis.

Poster T2-19

Antibiotic susceptibility of *Aeromonas hydrophila* monitored through SERS mapping methodology

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Abstract. The bacterial strain (PI-88 and PAI-45) used in this study were isolated from surface water of Cluj County (Romania) and further identified based on 16S rRNA molecular markers, using 27FB-1492R primer pair. Antibiotic susceptibility was carried out by disk-diffusion assay using six antibiotics as follows: Ampicillin (Amp), Carbenicillin (Cb), Oxacillin (Oxa), Penicillin G (Pen), Azlocillin (Azl), and Tetracycline (Tet). The SERS fingerprinting focused on identification of specific marker bands of the same bacterial strain in antibiotic treated and untreated samples. Based on inhibition zone diameter, the selected antibiotics showed antibacterial activity with variable magnitudes. Both *Aeromonas* strains were resistant to Ox and Pen and exhibited susceptibility to Tet and Azl, except PI-88 which expends susceptibility to Amp and Cb.

Poster T2-20

Allicin: natural distribution, antioxidant and biological activity profile

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Abstract. *Allium* species contain high amounts ofallicin, flavonoids as well as other antioxidant natural compounds. The most important class of bioactive compounds in *Allium* is represented by organosulphurous compounds which include allin, allicin, ajoene and some allicin-related degradative products.Our study aims to determine a phytochemical pattern of several *Allium* species (*A. cepa, A. obliquum, A. senescens* ssp. *montanum*, *A. urisinum, A. schoenoprasum*).In order to examine the antioxidant activity, we investigated the free radical scavenging activity by DPPH bleaching assay, TEAC assay and Folin-Ciolcâlteu method for hydrophilic antioxidants quantification. Allicin have been determined by HPLC method.The hydroalcoholic extracts of studied *Allium* species present a high diversity regarding antioxidant vs pro-oxidant activities. Allicin content showed that *A. obliquum* and *A. cepa* var. Roşie de Arieş are the richest extracts in thiosulphinates. Antioxidative and pro-oxidative activities are correlated with the concentration of polyphenols and thiosulphinates. Concerning the biological activities of *Allium*, there are a large spectrum of applications, including autism-like disorders.

Poster T2-21

Crystal and molecular structure of Sodium (2-carbamoylphenoxy) acetate

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Abstract. Sodium (2-carbamoylphenoxy) acetate is a compound with analgesic effects. A suitable 0,6 x 0,5 x 0,4 mm crystal, transparent was selected and analyzed on SuperNova diffractometer using Cu microsource and an Eos CCD detector. The crystal was kept at room temperature during data collection. The crystalline structure was solved using Olex2, with the ShelXS structure solution program and refined with ShelXL refinement package by least Squares minimization. The crystals of Sodium (2-carbamoylphenoxy) acetate $C_{36}H_{34}N_4Na_4O_{17}$ fit into P-1 space group of the triclinic crystallographic system with the following unit cell parameters: a = 10,8538(4), b = 13,6231(6), c = 13,8545(6), α = 103,770(4), β = 103,723(3), γ = 100.065(3), Z = 2, V = 1873Å^3. Other data like bond lengths, angle measurements and torsion angles were determined as well. For a better understanding of the intermolecular interactions which stabilize the crystalline structure, Hirshfeld surface was generated using Crystal Explorer software.

Section T3:

Energy Efficiency and High-Tech Engineering

Oral T3-1

Analysis, modelling and simulation of the Stirling engine functioning in real conditions

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Abstract. In this contribution, a thermo-technical analysis of the Stirling engine is carried out on the basis of thermodynamic quasi-real concepts. Analysis and modeling is performed for the five main regions: compression and expansion chambers, cooler, heater and regenerator by taking into account the real geometry of them. The void volumes are determined by geometrical shape of the cooler and heater as tubular, smooth pipes, annulus or slots. Additionally, the regenerator geometry can be considerate as a matrix having mesh as wire netting or wrapped foil configuration. Based on mass and energy conservative laws, a system of eight first-order ordinary differential equations has been developed. Equations system solutions are process as numerical functions defined in the [0 2π] range, such as pressure, fluid mass, cold and hot source temperatures, compression and expansion chamber energies as well as overall assembly performance. All of these are determined on the basis of an integrated computation code developed in the programming languages Gnuplot 5 and Maple 11 using Fourth Order Runge-Kutta algorithm. Effective power and efficiency changes will also be analyzed based on the pressure losses that occur during the Stirling engine cycle.

Oral T3-2

An Introduction to 1W1B-XAFS Station of BSRF

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Abstract. 1W1B-XAFS sation is a X-ray absorption fine structure beamline operating in the 4-25 keV range, which locates at Beijing Synchrotron Radiation Facility (BSRF). The energy range of the incident X-ray is tunable from 4 to 25 keV by fix-exit Si (111) double crystal monochromator. It supports trace element analysis (as lower to 10ppm) and extreme conditional experiments (such as high pressure (20GPa), high temperature (1073K) and low temperature (10K). In addition, electrochemical experiments can also be carried out, this is the hot topic on 1W1B recent years. It could run both in the dedicated mode of synchrotron radiation and in the parasitic mode. Every year, researchers from several disciplines work on it, such as physics, materials, environment and so on.

Oral T3-3

Hydrogen, an alternative fuel for energy efficiency in mobility

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Abstract. The hydrogen utilization as a non-polluting fuel for mobility requires a huge and complex human and material activity in the coming years as well as active cooperation at national level. There are both aspect technical, such as problem of safety production, distribution, utilisation, etc., and legislative framework. In Romania, the research groups like ICSI Rm. Valcea or ITIM Cluj-Napoca have a long tradition to promote the hydrogen as an alternative fuel for energy efficiency in mobility. The presentation wants to indicate the efforts made by these two groups of researchers over time.

Oral T3-4

Microwavable Mantle

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Abstract. Internally-heated convection has reached less attention that Rayleigh-Bénard convection although the decay of long lived radioactive elements (^{238}U, ^{235}U, ^{232}Th, ^{40}K) represents the most important heat source in the mantle of telluric planets. The initial concentration of radioactive elements in the bulk silicate Earth is poorly constrained and their distribution is heterogeneous: chemically distinct layers mark its top and its bottom. We have developed a new technology to produce internally-heated convection based on microwaves absorption. Our microwave-based method offers new perspectives for the study of internally-heated convection in heterogeneous systems which have been out of experimental reach until now. It allows the accurate study of mixing processes. We are able to selectively heat specific regions in the convecting layer, through the careful control of the absorption properties of different miscible fluids. This is analogous to convection in the presence of chemical reservoirs with different concentration of long-lived radioactive isotopes. Applied to a two-layered system of fluids designed to mimic the internally heated convection of a depleted mantle on top of an enriched denser reservoir, this technique provides insightful information on the generation and evolution of large low-shear-velocity provinces.

Oral T3-5

Optimization of positive electrode in lead-acid batteries: from design to experimental tests

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Abstract. The positive electrode in lead-acid batteries is one of the most sensitive parts of the whole battery, since it is affected by various aggressive chemical processes during its life. Therefore, an optimal design of the positive electrode of the battery may have as effect a dramatic improvement of the battery's properties - such as total capacity or endurance during its life. Our effort dedicated to this goal covers a range of rather complex tasks, from the design based on numerical analysis to tests on the working model, including the development of new investigations techniques. As result, we present several guiding rules form the electrode's design, together with the elements proving their validity, as indicated by experimental tests.

Oral T3-6

Working gas influence on the Stirling engine efficiency

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Abstract. Recently, there is an exponential growing interest in the use of alternative energy sources, due to excessive pollution and to cover the increase in global energy demand. One of the alternative ways to produce energy according to the new international regulations and environment friendly is by using a Stirling engine. In the past decade, the Stirling engine returned to the attention of scientist because of its great advantages. The big advantage of a Stirling engine is that it can produce electricity from clean renewable energy like solar energy and biogas. The Stirling engine operates by cyclic compression and expansion of air or other gas at different temperatures. Its efficiency directly depends by ratio of volumes, working temperatures and specific heat capacities of gas under constant volume and constant pressure conditions. For this study, we evaluated the influence of using mono-, bi- and triatomic gases as well as their mixtures on the efficiency of Stirling engine. Our contribution will furnish a reliable analytical analysis regarding the heat capacities of different gas types used in efficiency of the Stirling engine.

Oral T3-7

Hydrogen storage capacity of IRMOF-1 under applied electric fields

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Abstract. Hydrogen can be stored at high densities in metal-organic frameworks (MOFs) at low temperatures. MOFs are highly porous, with up to nanometer size pores and extremely large internal surface area (~5000m2/g). But, the performance of MOFs deteriorates at room temperature. This is due to the weak van der Waals forces responsible for the adsorption of hydrogen molecules on the pore walls. To address this roadblock, it was recently proposed to apply polarizing external electric fields and exploit the polarization effects to enhance the binding of hydrogen. Based on the state-of-the-art methodology, we develop a multiscale simulation tool for the hydrogen adsorption in metal-organic frameworks under the influence of applied electric fields. Our simulation tool allows us, for the first time, to make quantitative predictions of the hydrogen storage capacity of metal-organic frameworks subjected to an applied external electric field. We compute the adsorption isotherms for IRMOF-1 in electric field. While the improvement of adsorption is modest in this case, even for large applied fields, we show that substantial increase in adsorption capacity will occur if MOF's polarizability increases.

Poster T3-1

Raspberry Pi NIR camera with intervalometer

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Abstract. The intervalometer is an attachment or facility on a photo-camera that operates the shutter regularly at set intervals over a period. Professional cameras with built in intervalometers are expensive and quite difficult to found. The Canon CHDK open source operating system allows intervalometer implementation on Canon cameras only. However, finding a Canon camera with NIR photographic lens at affordable price is impossible. On experiments requiring several cameras (used for measure growth in plants - the crescographs, but also for coarse evaluation of the water content of leaves), the costs of the equipment's are often over budget. Using two Raspberry Pi modules equipped each with a low cost NIR camera and a WIFI adapter (for downloading pictures stored on the SD card) and some freely available software we have implemented two low budget intervalometer cameras. The shutting interval, pictures number to be taken, image resolution and some other parameters can be fully programmed.

Poster T3-2

Anisotropic electronic transport in layered calcium cobaltite $Ca_3Co_4O_9$

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Abstract. Thermoelectrics are promising to address energy issues but full potential exploitation requires improvements in their performance (high power factors and low thermal conductivities). We showed recently that highly anisotropic flat-and-dispersive electronic bands can maximize the power factor as long as these anisotropic bands have significant weights on transport and the carrier mobilities along transport direction have high values. These very anisotropic bands can create low-dimensional electronic transport even in bulk materials. Using first-principles calculations, we studied the electronic and thermoelectric (TE) properties of layered $Ca_3Co_4O_9$, known as a potential p-type TE oxide material. We find B1-WC hybrid functional to be appropriate for describing the structural, electronic, and TE properties of $Ca_3Co_4O_9$. These properties show a strong in-plane anisotropy. The qualitative behavior of the averaged in-plane properties is consistent with the measurements reported in the literature.

Poster T3-3

A power saving protocol for impedance spectroscopy

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Abstract. Because power saving is a main concern of wearable devices we present here a transient method with a low power demand for impedance spectroscopy of the skin, but the idea is valid for other test materials. The used signal is an electrical pulse (width T, the ON period) followed by a pause (the OFF period) when the electrodes do not receive or transmit current (high impedance status). The method has the advantage of being able to measure at once the frequency characteristics of the impedance and is well suited to obtain the bioimpedance which changes in time. Also, this kind of measurement creates a more direct and explicit relationship between lumped elements of the electrical model and measured signal.

Poster T3-4

Solar energy conversion on a two-axis tracker

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Abstract. Together with hydro and wind powers, solar energy is the most important renewable energy source in terms of globally capacity. In this respect, we designed an in-house two-axis tracking system containing both photovoltaic panels and Fresnel lenses as solar concentrator. We used Peltier elements to convert the concentrated solar energy to electricity. A total of 12 Peltier elements were installed with a maximum power capacity of 250 W and two photovoltaic panels with a maximum power of 490 W. The aim of the study was to compare the conversion efficiency of photovoltaic panels versus concentrated solar energy system per square meter irradiated surface.

Poster T3-5

Photothermal characterization of liquid thermoelectrics

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Abstract. Two alternative optothermal methods are proposed for thermal characterization of liquid thermoelectrics (LTE). The first method is a combined photopyroelectric-photothermoelectric (PPE-PTE) technique, coupled with the thickness scanning (TWRC) procedure. The PPE-TWRC technique, in back detection configuration leads to the direct measurement of the LTE's thermal diffusivity. Simultaneously, the PTE-TWRC method, in front detection configuration, is used for the measurement of LTE's thermal effusivity. The second alternative is also a combined PPE-PTE technique, but coupled with both thickness and chopping frequency (FS) scanning procedures. The PPE-TWRC technique, in back detection configuration is used to the direct measurement of the LTE's thermal diffusivity. Based on the results obtained for thermal diffusivity, two PPE-FS scans, performed at two different thicknesses are used for the precise determination of absolute LTE's thicknesses. Simultaneously, PTE-FS scans, performed at the same thicknesses, lead to the value of LTE's thermal effusivity. The results, obtained on a well-known LTE (octanol + TDAN) are in good agreement with previously reported data.

Poster T3-6

The role of hydrogen as a future solution to energetic and environmental problems for residential buildings

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Abstract. The concept of sustainable development aims to satisfy the needs of the present without compromising the needs for future generations. In achieving the desideratum "low-carbon energy system", in the energy production domain, the use of innovative low-carbon technologies is required, to provide maximum efficiency and minimum pollution. An example of such technology are the fuel cells, to obtain hydrogen based energy. Thus, hydrogen produced by electrolysis of water using different forms of renewable resources becomes a secure and sustainable energy alternative. In this context, in the present paper a comparative study of two different hybrid power generation systems for residential building placed in Cluj – Napoca was made, that integrate renewable energies (photovoltaic panels and wind turbine), backup and storage system based on hydrogen (fuel cell, electrolyser and hydrogen storage tank), respective backup and storage system based on traditional technologies (diesel generator and battery). The software iHOGA was used to simulate the operating performance of the two hybrid systems. The aim of this study was to compare energy, environmental and economic performances of these two systems and to define possible future scenarios of competitiveness between traditional and new innovative technologies. After analyzing and comparing the results of simulations, it can be concluded that the fuel cells technology and hydrogen joint undertaking, integrated in a hybrid system, may be the key to energy production systems with high energy efficiency, making it possible to increase the yield capitalization of renewable energy with a low environmental impact.

Poster T3-7

Pulsed laser deposition of Fe-based Heusler compounds for thermoelectric applications

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Abstract. The aim of the work was to grow thin films of Fe-based Heusler compounds on magnesium oxide (MgO) substrates using pulsed laser deposition (PLD). First, a buffer layer of MgO has been deposited and optimized by PLD onto Si(100) substrates, with the preferential orientation (100). Then, Fe-based Heusler compounds have been deposited onto MgO(100), using as targets bulk intermetallic Fe/Ti/Si/Sn compounds, with known stoichiometry. By optimizing the deposition parameters, it is possible to control the stoichiometry and crystallinity of the films, the properties of Heusler compounds being very sensitive to crystal structure disorder. The structural and morphological properties of the thin films thus obtained (morphology, preferred orientation, thickness, crystallinity) were investigated by XRD and SEM. Fe-based Heusler compounds are promising candidates for thermoelectric devices.

Poster T3-8

Influence of the Cu doping on the Electronic Structure and Magnetic Properties of the Mn_2VAl Heusler compound

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Abstract. Detailed investigations on the electronic and magnetic properties of the Heusler compounds $Mn_{2-x}Cu_xVAl$ (x = 0, 0.1, 0.2, 0.5) with $L2_1$ structure have been performed. The $Mn_{2-x}Cu_xVAl$ ingots were prepared by induction melting of the high purity starting components (> 99.9 %) under a purified Ar atmosphere. The resulting polycrystalline samples have been studied by X-ray diffraction (XRD) and magnetization measurements. The degrees of the B_2 and $L2_1$ atomic ordering were obtained by using the Takamura's extended order model [1] for Heusler compounds from the XRD patterns. The Curie temperatures decrease with increasing Cu content, ranging between 771 K (x = 0) and 580 K (x = 0.5). Additionally, electronic band structure calculations using the Korringa-Kohn-Rostoker (KKR) Greens function method have been performed. The substitutional disorder was accounted by the means of the Coherent Potential Approximation (CPA). The site occupation considered in the calculations has been correlated with those obtained by the XRD experiments. Our study gives insight on the evolution of the half-metallic fully compensated ferrimagnet (HMFi) character with disorder and Cu doping showing restrictions in the obtaining of a HMFi by doping with 3d metals.

Poster T3-9

Finite element optimization of a heat pump based on electrocaloric effect

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Abstract. Refrigeration is one of the main source of energy consumption and greenhouse gas emissions in the word. In recent years there has been an upsurge of interest in high efficiency alternative cooling technologies which are more environmentally acceptable then traditional vapor-compression refrigeration systems (VCR). Caloric materials seem to be new refrigeration solutions able to replace current VCR. Electrocaloric materials undergo an adiabatic temperature change (heating-up/cooling-down) when an electric field is applied or withdrawn, respectively. This work focuses on the demonstration of the conceptual operation of caloric refrigeration or heat pumping. We present a physical model that analyzes the key parameters for performance optimization of a system driven by heat switches. A thin electrocaloric material was coupled with two thermal switches. The thermal switches were designed as an alternative transfer fluid/air motion. To model the flow of heat through the proposed multilayer system, we used the finite element analysis (Comsol Multiphysics). We numerically calculated the effect of parameters (frequency, thickness of EC material, the phase shift) in heat transfer efficiency. The maximum temperature change was $\Delta T_{max} \cong 0.6^0C$. The model shows benefits for optimization and design of real heat pumps.

Poster T3-10

Ferroelectric Metal-organic Frameworks for Energy Storage

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Abstract.

Electric fields have the potential to markedly improve the hydrogen adsorption on high surface adsorbents such as nanosheets of graphene, boron nitrates and aluminium nitrates. Despite MOFs (metal-organic frameworks) being the most promising systems for hydrogen storage based on physisorption, there are no studies concerning the influence of the electric field on the adsorption of hydrogen in these systems. One of the reasons for this is that the proposed electric fields are too large and can cause Zener breakdown in MOFs. However, based on our calculations, even relatively low electric fields can improve significantly the adsorption, if MOFs are highly polarisable. We propose a class of polarisable MOF materials belonging to the ferroelectrics. We selected two compounds based on their high porosity, pore volume, crystalline density and crystallographic space group which were synthesized and characterized with the intention to experimentally test hydrogen adsorption in electric fields.

Poster T3-11

Brief Introduction – Photoemission spectroscopy (PES) Beamline @BSRF

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Abstract. A brief introduction to the photoemission spectroscopy (PES) beamline at Beijing Synchrotron Radiation Facility (BSRF). The PES beamline locates at 12# experimental hall in the Institute of High Energy Physics (IHEP), Chinese Academy of Sciences (CAS). It is based on a bending magnet light source which is dedicated to x-ray photoemission spectroscopy (XPS) and soft x-ray absorption spectroscopy (XAS) studies, which can further focus the beam to a size of 2 mm x 0.8 mm. The X-ray energy is from 20~ 1000eV. The research of this beamline focuses on material science, condensed matter physics fields, surfaces and interfaces, nano-materials.

Poster T3-12

Small-Angle X-ray Scattering Study on Electric Response of Electrorheological Fluid

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Abstract. 1W2A is the small-angle X-ray scattering (SAXS) beamline of the Beijing Synchrotron Radiation Facility in the Institute for High Energy Physics (Beijing, China). The beamline was opened to the scientific users in 2007. SAXS techniques have been widely applied in diverse research fields, such as material science, chemistry and biomedicine. Our latest work is the in-situ study on electric response of electrorheological (ER) fluid which is the mixture of nano particles and silicone oil. When an electric field is applied, disordered nano particles in oil would align alone the field direction. This disorder- order transformation is reversible when canceling electric field. The orientation and aggregation of particles caused by electric field could be researched intensively by adoption of in-situ SAXS data. This research would provide new experimental basis for theory of ER fluid.

Poster T3-13

Laser-atom interaction beyond the strong field approximation model

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Abstract. The most accurate theoretical methods for investigating the laser-matter interaction rely on the 'exact' solution of the time-dependent Schrödinger equation (TDSE), however these methods request a high amount of computing time even for smaller systems, such as atoms or molecules considered of having a single active electron (SAE approximation). In order to less expensively calculate the single atomic (molecular) responses of the irradiated systems, and to obtain in a shorter time the HHG spectra generated through the macroscopic medium, the Strong Field Approximation method was developed, which has been widely applied in the recent years. Even though the SFA is considered a good tool for such fast calculations, recent studies in the short-wave infrared domain showed divergences between the predictions of this model and the exact results. In order to eliminate these divergences J.A. Pérez-Hernández et al. proposed an extended version of the SFA model. In this work we implemented the extended method of SFA (referred here as SFA+), which in addition to the simple model can also take into account field dressing and the recollision step through the electronic bound states, at the same time it eliminates the major deficiencies of the former method. We also extended our calculations for the cases of different synthesized wave forms obtained by experimentalists.

Poster T3-14

Attosecond lighthouse generated with shaped mid-infrared laser pulses

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Abstract. When temporally short (~10^{-15} s), very intense (~10^{14} W/cm^2) mid-infrared (MIR) laser pulses propagate in dispersive and highly ionizing medium (e.g. rare gas) we expect that a dynamic rotation of the wave front occurs due to the rapid variation of the medium's refractive index. It is possible to use such a wave front rotated laser pulse as fundamental for high-order harmonic generation in order to obtain coherent XUV radiation. The properties of the fundamental MIR are transferred to the up-converted frequencies, therefore the harmonics generated with increasing divergence in successive optical cycles of the MIR, will be detected at increasing distances from the optical axis in the far-field. The radial separation of the successive XUV emissions is called the attosecond lighthouse. Its advantage comes from the fact that the radially separated XUV bursts appear as isolated attosecond pulses, and these can be further used in attosecond pump-probe experiments without additional spectral or temporal filtering, preserving in this way the total flux of the radiation. In this paper, we explore different possibilities to enhance and improve the lighthouse effect by shaping the initial MIR pulse, for example induce a controlled amount of linear chirp. The expected results are both higher XUV flux at the outcome and better radial separation of the successive XUV bursts.

Poster T3-15

Considerations for designing robotic upper limb rehabilitation devices

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Abstract. The present study highlights the advantages of post-stroke rehabilitation of the upper limb using robotic systems. The latest demographic studies illustrate a continuous increase of the average life span, which leads to a continuous increase of stroke incidents and patients requiring rehabilitation. Some studies estimate that by 2030 the number of physical therapists will be insufficient for the patients requiring physical rehabilitation, imposing a shift in the current methodologies. A viable option is the implementation of robotic systems that assist the patient in performing rehabilitation exercises, the physical therapist role being to establish the therapeutic program for each patient and monitor their individual progress. Using a set of clinical measurements for the upper limb motions, the analysis of rehabilitation robotic systems provides a comparative study between the motions required by clinicians and the ones that robotic systems perform for different therapeutic exercises. A critical analysis of existing robots is performed using several classifications: mechanical design, assistance type, actuation and power transmission, control systems and human – robot interaction (HRI) strategies. This classification will determine a set of pre-requirements for the definition of new concepts and efficient solutions for robotic assisted rehabilitation therapy.

Poster T3-16

An experimental reactor for bioethanol production

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Abstract. A miniaturized biochemical reactor meant to produce ethanol from liquid solutions containing mainly water dissolved polysaccharides is reported herein. The reactor is aimed for studying the influence of the chemical composition of the broth and the influence of the external factors (temperature, light, etc.) that may influence the bioethanol yield. The main envisaged biochemical reaction is supposed to be carried out by Saccharomyces Cerevisiae strains. The proposed reactor is developed in order to accommodate a small quantity of liquid reaction medium (about 10ml), while providing the paths for feeding the reaction chamber and sampling the liquid. The reactor is meant for studying the influence of nanostructured materials over the broth composition with the aim to enhance the bioethanol yield as well as for testing various vegetal prime materials.

Poster T3-17

Water intake flow efficiency study for micro-hydro power plant

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Abstract. The water intake from the micro-hydro power plans capture water in two ways, namely, in summer through a surface grill and in winter by "winter intake", which is immersed in water below freezing level. The water flow captured for energy production is influenced by the river flow and fish ladder flow, respectively. The fish ladder flow should ensure a minimum servitude flow, downstream for fish migration. The paper presents a study concerning optimization of water flow capture for micro-hydro power plants in order to increase the energy production. This optimization should be made by keeping a constant flow though the fish ladder. The increase on the efficiency as a function of the river flow will be presented.

Poster T3-18

Innovative Cluster for Pilot Technology in Alternative Energy

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Abstract. Transylvania Energy Cluster – TREC is part of the TREC Danube - the transnational network of regional clusters in the field of renewable energy, energy systems and bioeconomy. We are linking networks, business partners and R&D organisations from Nord West Region of Romania – Transylvania Area. TREC is a platform for R&D driven innovations in alternative energy, renewables, energy efficiency and advance environmental technologies and environment protection. In our project – Innovative Cluster for Pilot Advanced Technologies in Renewables Energy – CITAT-E, we intend to build a demonstrative mixed alternative energy framework in the Cluj-Napoca area in order to show that combining these renewable sources a better energy efficiency will be obtained. By showing the results to the potential investors we consider that their trust in sustainable energy obtained by alternative sources will be increased and they will invest in this idea in the future. We will also build a mix energy platform which will be able to calculate the energy efficiency and this will give us the possibilities to give different solutions adapted with the climate condition and the necessities of different investors. During the project, we will improve the energy efficiency of this park by experience exchange between partners and the result will be compared in order to show which is the best solution for best energy efficiency and storage adapted with the area and the results we expect to obtain.

Poster T3-19

The assessment of global thermo-energy performances of existing district heating systems optimized by harnessing renewable energy sources

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Abstract. In the thermo-energy optimization process of an existing heating system, the increase of the system's energy efficiency and speeding-up the transition to green energy use are pursued. The concept of multi-energy district heating system, with high harnessing levels of the renewable energy sources RES in order to produce heat, is expected to be the key-element in the future urban energy infrastructure due to the important role it can have in the strategies of optimizing and decarbonizing the existing district heating systems. The issues arised are related to the efficient integration of different technologies of harnessing renewable energy sources in the energy mix and to the increase of the participation levels of RES, respectively. For the holistic modelation of the district heating system, the concept of the energy hub was used, where the synergy of different primary forms of energy entered provides the system a high degree of energy security and flexibility in operation. The optimization of energy flows within the energy hub allows the optimization of the thermo-energy district system in order to approach the dual concept of smart city & smart energy.

Poster T3-20

Broadband rectenna array for electrosmog harvesting

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Abstract. A wide frequency band (0.8GHz-12GHz) rectenna (rectifier antenna) array is presented. The array converts the electromagnetic (EM) energy to direct current (DC). The purpose of this broadband rectenna array was to clean up in its proximity the EM pollution – defined as electrosmog. The most common sources of EM pollution are related to the generic wireless applications as GSM, WI-FI, WLAN, etc. The array can be adapted well to any low power applications of EM energy harvester used for DC supply. The broadband rectenna array consists on 48 elements, grouped in 8 panels of 6 rectennas each, a total geometric area of $0.6m^2$. The rectenna itself is composed by a broadband microstrip antenna (circular polarisation) connected to a rectifier and a voltage doubler (patent pending, RO131697/2016). Each of the 8 panels it is a printed circuit board (PCB) with the 6 DC rectenna outputs connected in series. One panel it is a DC source delivering 1V for an EM power density of $1mW/m^2$. Our goal is to harvest 1mWh of energy for discontinuous supply of low power application such as a sensor connected to a data logger. The measurements validate the goal by harvesting lower than $25mW/m^2$ electrosmog power field density.

Poster T3-21

Efficient low-power wireless communication setup for an autonomous soil moisture sensor

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Abstract. During July 2016 - September 2017, a micro-irrigation system was set up and tested in field and greenhouse-like conditions, using eight inexpensive soil moisture sensors designed and manufactured in our institute. Each sensor was powered by accumulators charged by an (8×14) cm^2 solar panel. The energy budget was carefully managed to allow long operating time for both the moisture sensor and the irrigation automation. We present here the hardware-software setup implemented in our proprietary moisture sensor for wireless communication (60m Line Of Sight-LOS), using Bluetooth Low Energy modules (BLE). The autonomy of the system may reach 4-5 cloudy days without the need of recharging the accumulators from the sun. Over the entire operating period, the moisture sensors send data wirelessly every 30 minutes and water drips on the soil for the next 30 seconds, pushed by a low power micro-pump. The micro-irrigation process is repeated every 30 minutes, until the soil moisture threshold is reached. In between the operating states, the sensor and watering automation go to sleep. The software algorithm ensures low energy (max. 2.8 mWh) consumption for the moisture sensor and 20 mWh for the irrigation automation, substantially increasing the accumulators discharge cycle.

Poster T3-22

A spectral image processing algorithm for evaluation the influence of the illuminants on the reconstructed reflectances

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Abstract. A spectral image processing algorithm that allows the illumination of the scene with different illuminants together with the reconstruction of the scene's objects reflectances is presented. Color checker spectral image and CIE A (warm light 2700 K), D65 (cold light 6500 K) and Cree TW Series LED T8 (4000 K) are employed for scene illumination. Illuminants used in the simulations have different spectra and, as a result of their illumination, the colors of the scene change. The influence of the illuminants on the reconstruction of the scene's refectances is estimated. Demonstrative images and reflectances showing the operation of the algorithm are illustrated.

Poster T3-23

Femtosecond pulse propagation and harmonic generation in multiple ionizing media

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Abstract. Ultrashort pulse propagation in gas media is numerically studied for pulses of 20-40 fs duration and peak intensities from 10^{15} to 10^{17} W/cm^2. In these conditions, the (usually noble) gas suffers multiple ionizations in a sequential manner, giving rise to highly charged species, for ex. Ne, Ne^+, Ne^{2+}, up to a complete stripping of the atom, Ne^{18+}. The complex plasma medium is studied in view of its capacity to emit harmonics. Indeed, ionization processes are followed by (much less efficient) recombination events in which the kinetic energy of the electrons, accumulated during their trip outside atom/ion, is converted in a single photon of high energy, ranging from VUV to soft x-ray. A previously existing model, dealing with single ionization case, was developed further on to include propagation effects in these conditions and harmonic generation by the different ionic species. The results are discussed in connection with experimental data obtained in other laboratories.

Poster T3-24

Coupled photothermal methods for thermal characterization of solid thermoelectrics

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Abstract. The dynamic thermal parameters (thermal diffusivity and effusivity) of four solid thermoelectric materials (ZnO, TiS_3, $CuCrO_2$, $Cu_4Sn_7S_{16}$) have been investigated by using two photothermal techniques: the photopyroelectric (PPE) and the photothermoelectric (PTE) methods. The value of the thermal diffusivity was measured by using both methods in back detection configuration with a $LiTaO_3$ (PPE) and $CuCrO_2$ (PTE) sensors, respectively. The thermal effusivity was measured in the front detection configuration by using the thermoelectric material as a sensor. The results obtained by both photothermal methods are in good agreement.

Poster T3-25

Brief Introduction of 1W1A Diffuse X-ray Scattering Beamline @BSRF

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Abstract. 1W1A is a diffuse X-ray scattering beamline operating at 8.05 keV and 13.9 keV, which locates at I quadrant of BEPC and 12# experimental hall, which can focus the beam to a size of 0.7mm x 0.4 mm with flux >1 x 1011(photons/sec)@8.05keV. It supplies double focusing monochromatic light and supports the structure researches on crystal and thin-film materials. It could run both in the dedicated mode of synchrotron radiation and in the parasitic mode. Supported techniques include: Coplanar X-ray diffraction/ scattering, Grazing incidence X-ray diffraction/scattering, X-ray reflectivity/Non-specular X-ray scattering, Grazing incidence small angle X-ray scattering (GISAXS) etc.

Section T4:

Nanostructured Materials - Nanocomposites and Hybrid Materials

Oral T4-1

Monitoring the effect of silica fume on the pore evolution of cement paste via Fast Field Cycling NMR relaxometry

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Abstract. Silica fume is a popular mineral admixture used in the development of high performance concrete. As a pozzolanic material available in powder form, with sub-micron particle sizes, it is useful both for increasing the mechanical strength of concrete and for filling the capillary pore system, including the cement-aggregate interfacial transition zone. In the present work, the effects introduced by silica fume on cement paste hydration and pore system development were investigated using the non-invasive nuclear magnetic resonance (NMR) relaxometry. Thus, the development of the pore system in hydrating cement pastes with increased amounts of silica fume was monitored via Fast Field Cycling (FFC) relaxometry. It was observed that during the first ten hours of hydration there is a systematic acceleration of the hydration kinetics by increasing the amount of silica fume. Moreover, a reduction in the size of capillary pores was detected from FFC relaxation data. This will influence not only the final strength of the manufactured materials but also their permeability. The outcomes of our studies may help the development of new cement-based materials with higher durability and increased long-term mechanical resistance.

Oral T4-2

Revealing the Influence of Water-Cement Ratio on the Pore Size Distribution in Hydrated Cement Paste by Using Cyclohexane

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Abstract. Varying the amount of water in a concrete mix will influence its final properties considerably. A non-destructive technique for revealing the capillary pore distribution inside hydrated cement based materials is necessary for linking the capillary porosity with the macroscopic properties of these materials. This paper introduces an easy to use method of revealing the differences in capillary pore size distributions between cement pastes with different water-to-cement ratios. It applies a common NMR technique, the CPMG echo train acquisition, on samples filled with a neutral nonpolar solvent, cyclohexane, which does not dry the sample, nor react with the hydration products. The technique reveals the whole spectrum of pores inside the hydrated cement pastes, allowing a qualitative and quantitative analysis of different pore sizes. The cement pastes with higher water-to-cement ratios show an increase in capillary porosity, while the intra-C-S-H and inter-C-S-H pores (also known as gel pores) remain unchanged. The technique can be applied to various porous materials with internal mineral surfaces.

Oral T4-3

The interaction of hydrogen with nanosized Pd clusters

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Abstract. Sizing of metals at nano level become rapidly a promising route used to design new materials with applications in fields like energy storage, catalysis, sensing etc. A way to obtain and stabilize metal nanoparticles against coalescence and the subsequent formation of large aggregates with bulk-like behaviour is to use nanoporous scaffolds like metal-organic frameworks. The present work reports the synthesis and properties of hybrid materials obtained dispersion of Pd nanoparticles within the MIL-101 pores. Experimental results revealed that hydrogen absorption kinetics and thermodynamics are significantly modified by nanosizing.

Oral T4-4

Do small defects in surfaces affect the molecular electronics? The DFT approach

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Abstract. In the quest for better and cheaper electronics, many organic molecules with good conduction properties, such as Phthalocyanines (PCs) hosting metallic ions were introduced as building blocks in nanotechnology. In addition to a cheap and reliable molecule to form the active layer, also the metallic substrate should possess good properties and low price. Since the high-quality surfaces have prohibitive prices and the lab-made substrates have inherent small defects, the question that arises is how important is the surface quality in the nanodevices construction. We thus fabricated a substrate by covering the reconstructed 7×7 Si(111) with Au using the MBE technique. This surface was further used for depositing FePC at low rate, to investigate the molecule's adsorption characteristics. In this respect, we investigated the surface corrugation and the point-like defects, consisting in atom-sized holes in surface by both STM and a three-scenario computational approach. This investigation resulted in a comprehensive characterisation of the FePC interaction with the lab-constructed surface. We showed that the molecule preserves its conductive properties regardless the substrate integrity.

Oral T4-5

Electrochemical sensors based on molecularly imprinted polymers for antibiotics detection

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Abstract. There is a noticeable increase in the use of biopolymers and synthetic polymers in medicine and pharmaceutical analysis as drug delivery and therapeutic systems, macromolecular prodrugs, as well as biomimetic receptors and recognition element. By using molecular imprinting technique, it is possible to create robust tailor-made polymers for specific target molecules. Molecularly imprinted polymers possess quite unique and attractive features such as selectivity comparable to that of affinity biomacromolecules and a remarkable stability under various experimental conditions. The antibiotics represent one of the most important therapeutic classes, but their misuse and overuse in human and veterinary medicine have resulted in the increased number of allergies and in the development and spread of antibiotic resistance. Antibiotic resistance has a significant impact on health and economy, WHO recommending an urgent improvement in the surveillance of the use of antibiotics, hence the need for developing new analytical sensors, capable to detect selectively low concentrations of antibiotics from different matrices. The purpose of this study was to develop electrochemical sensors for the detection from environmental and pharmaceuticals samples of β-lactam and macrolide antibiotics, two widely used antibiotic classes.

Oral T4-6

Effect of porosity on the dielectric and dc-tunability properties of $BaTiO_3$ ceramics

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Abstract. Materials with controlled porosity exhibit special properties that usually cannot be achieved by their conventional dense counterparts. Porous materials find nowadays many applications especially for environments where high temperatures, extensive wear and corrosive media are involved as well as for advanced applications as piezoelectric and energy harvesting device. The functional properties of the porous ceramics can be tailored for each specific application by controlling the composition, type of porosity (open or closed), pore size distributions, pore morphology and interconnectivity. Starting from this idea, our theoretical approach based on Finite Element Method (FEM) calculations demonstrated that porous ferroelectrics might show promising tunability properties for applications in wireless technology. Using this approach, we proved that the case of porous ferroelectrics with closed porosity is the best solution to fulfil the tunability requirements (low losses: tan $\delta < 3\%$, moderate permittivity $\varepsilon < 1000$). The aim of the present work was to investigate in a systematic way the role of the pores concentration and phase interconnectivity (0-3, 3-3 and 1-3) on the functional properties of $BaTiO_3$ porous ceramics. The obtained results show that by increasing porosity a systematic reduction of permittivity was obtain, while the tunability is almost constant. The results were explained using the concept of local field engineering, in order to propose new porous configurations with improved tunable properties.

Oral T4-7

High pressure hydrogen adsorption on MIL-101

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Abstract. On-board hydrogen storage for applications to fuel-cell based vehicles is one of the most challenging barriers for commercialization. To reach the required hydrogen storage density of 40 g/L, high pressure 70 MPa storage cylinders currently developed are used. High temperatures are developed inside the tank during charging, which is a drawback together with the risk implying a high pressure. The decrease of storage pressure has been a continuous concern and this can be achieved using sorbents which could store high amounts of hydrogen in molecular state by physisorption in cryo-adsorption conditions at temperatures which could be higher as compared to liquid and cryo-compressed options. At low pressure, there is a significant gain as compared to the volumetric capacity of the empty cylinder. However, as the pressure increases, this gain diminishes and eventually it becomes zero at this "break-even pressure". For various hybrid storage methods proposed, additional data on the hydrogen adsorption isotherms of the sorbent in the range of interest 150-200K are required. Original data on the adsorption isotherms for MIL-101 are reported, a metal-organic framework with good sorption properties, currently synthesized by our group.

Oral T4-8

Superconducting $YBa_2Cu_3O_{7-\delta}$ nanocomposites using ZrO_2 colloidal solution obtained by polyol route

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Abstract. The incorporation of additional nanoscale inhomogeneities into $YBa_2Cu_3O_{7-\delta}$ (YBCO) matrix represents a new approach in the CSD-based YBCO films. Superconducting YBCO nanocomposites are fabricated via chemical solution deposition (CSD) using ZrO_2 nanocrystals. ZrO_2 nanocrystals have been synthesized in liquid polyols at elevated temperature. The nanoparticles are stabilized in an alcoholic solution, either through the initial use of solvents, also behaving as ligands, or through ligand exchange. The structure and morphology of the nanoparticles were studied using XRD, TEM, and FTIR. The ZrO_2 nanoparticle suspension has been subsequently mixed and stabilized in the metal–organic trifluoroacetate precursor solution, used for YBCO film growth, to form a stable colloidal solution with the desired concentration. By using these solutions, epitaxial c-axis oriented YBCO nanocomposite layers have been obtained. The influence of the ZrO_2 content on the superconducting properties of YBCO – ZrO_2 nanocomposite films has been studied. Improved transport properties have been recorded for the low ZrO_2 nanoparticle concentration nanocomposite films. The morphology of the nanocomposite films is slightly influenced by the amount of nanoparticles incorporated into the system.

Oral T4-9

Shape-stabilized phase change materials with dual thermal response and high energy storage obtained using mesoporous silica matrices

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Abstract. Phase change materials (PCMs) can reversibly store thermal energy for various applications, such as low-grade heat recovery and solar thermal storage. Due to the high molar volume change during phase transition, pure PCMs exhibit several disadvantages (leakage, decrease thermal transfer and storage), which can be alleviated by impregnation in high porosity matrices or encapsulation. Mesoporous silica nanoparticles (MSN) are a promising matrix for PCMs, offering high porosity, chemical and thermal stability. However, composite PCMs using mesoporous silica have typically had low heat storage capacity, due to the existence of an interfacial non-melting layer. We obtained composites using fatty acids as thermal storage medium and various mesoporous silica carriers and investigated the influence of silica textural properties and surface modification on the thermal properties. High storage materials can be obtained through a careful selection of mesoporous carrier properties. The nanocomposites show two separate operating temperature ranges, associated with intra-particle and nanoconfined PCM phases.

Oral T4-10

α-Hydroxy acids as bricks for functionalized polymers engineering

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Abstract. α-Hydroxy acids may be either naturally occurring or synthetic. Condensation products of α-hydroxy acids produced by self-esterification with the elimination of the water have been known for some time as polyesters. But the known polyesters have many limitations, often too hydrophobic for applications in aqueous environments, and more importantly, they lack chemical functionality that enables modification of the polymer backbone. Therefore, we targeted our work in developing some functional polymers starting from α-hydroxy acids. In this work, we report about the synthesis of some new functionalized polymers where we used α-hydroxy acids as starting monomers. The polycondensation of these monomers can take place or as a self-esterification but also in a special case as a poly-Friedel-Crafts alkylation. The polymers where characterized using NMR spectroscopy, ss-NMR spectroscopy, FTIR, mass spectrometry and SEM. The above-mentioned polymers were employed also to cover the surface of magnetic nanoparticles. The resulting magnetic nanostructures are characterized by various methods such as FTIR, X-ray photoelectron spectroscopy, transmission electron microscopy (TEM) and magnetic measurements.

Oral T4-11

Graphene synthesis through electrochemical exfoliation of graphite rod

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Abstract. Novel approaches for the synthesis of graphene nanosheets through electrochemical exfoliation of graphite rod in the presence of organic molecules (porphyrin) or TiO_2 nanoparticles are reported. The as prepared materials were fully characterized by TEM/SEM, FTIR, Thermogravimetric analysis and X-Ray powder diffraction. The main advantages of the synthesis methods consist in the excellent preservation of the 2D structure, good reproducibility in the number of layers and excellent adherence to the transducer surface (glassy carbon). The performances of the electrochemically exfoliated graphene (EGr) deposited on top of glassy carbon electrodes were also evaluated.

Oral T4-12

Design of micro-and nanostructured metallic films by direct laser writing

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Abstract. The novelty of our work is that controlled irradiation with pulsed UV laser radiation of a thin polymeric film doped with noble metal precursors allows to be obtained extended micro- and nanostructured metallic surfaces. Areas of well-defined geometries and sizes can be designed, without requiring the use of masks with dedicated shapes and sizes. Optical lithography by direct laser writing in thin films provides the adjustment of the metallic film's granulation at micron and submicron scale.

Poster T4-1

Fighting against bacteria colonies

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Abstract. Nosocomial infections (NIs) are a major concern for public health. As more and more pathogens responsible for these infections become antibiotic resistant, finding new ways to overcome this drawback is a major challenge for biomedical research. Despite strict hygiene standards, biofilm related infections are associated also with implantable devices, a common complication in hospitals. It is widely accepted that the most effective way to combat biofilm formation is *a priori* suppression of bacterial adhesion rather than *a posteriori* chemical- or drug-based treatment. We propose here viable methods and materials to reduce NIs spreading by hindering bacterial adhesion in its very early stage. Reducing the bacterium-surface contact area by surface engineering is a promising way to obtain bactericidal effect. We performed a systematic investigation of surface morphology influence upon preventing biofilm formation. In particular, two distinct approaches in surface microengineering have been compared: (i) surfaces patterned by nanoimprint lithography (NIL) and (2) polymeric surfaces with random morphology created by polymerization of dopamine. Efficiency in preventing biofilm formation and bacteria growth has been evaluated by microbiological tests.

Poster T4-2

Influence of the thermal treatment on structural properties of some zinc-phosphate glass doped with manganese ions

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Abstract. In order to describe the influence of thermal treatment on zinc-phosphate glass matrix doped with manganese ions, XRD and FT-IR measurements were performed. XRD patterns reveal that the crystallinity degree slowly decreases by increasing MnO content in the samples. Also, the FT-IR spectra confirm the fact that the glass network suffers some changes after thermal treatment. The spectra of thermally treated samples contain new peaks and the IR bands become narrow, compared to those of the untreated samples.

Poster T4-3

Effect of erbium(III) oxide addition on thermal properties and crystallization behavior of some zinc-borate glasses

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Abstract. The effect of replacement of B_2O_3 by Er_2O_3 on the thermal properties and crystallization behaviour of B_2O_3-ZnO glasses were investigated by DTA and XRD measurements. DTA measurements reveal that the temperature of vitreous transition and the glass stability increase with the increasing in concentration of erbium ions added in the samples. The fragility index of the glasses increases also, when the dopant concentration from the studied samples increase, the glass being approach by KS type glass. The most stable sample form the thermal point of view seems to be the sample that contain 10 mol% of Er_2O_3. The XRD patterns show new crystalline phases that contains erbium when the concentration of Er_2O_3 in the samples is higher than 3 mol%.

Poster T4-4

The role of gadolinium(III) oxide addition on structural and magnetic properties of some thermally treated zinc-borate glasses

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Abstract. RPE and magnetic susceptibility measurements were performed to determine the role of gadolinium ions (from Gd_2O_3 oxide) on structural and magnetic properties of thermally treated zinc-borate glass matrix. RPE data show that the disorder from the glass network increase with the increasing of the Gd_2O_3 content. The magnetic measurement reveals an antiferromagnetic behaviour for gadolinium ions in the glass network.

Poster T4-5

Ar^+ jet treatment, before deposition, and low substrate temperature, during deposition – factors which enhance the solid-state de-wetting of thin Au films

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Abstract. Temperature treatment of gold films deposited on glass substrates by thermal evaporation is known to induce the de-wetting of glass by the uniformly deposited gold film, leading to an island-like structure of gold on the glass substrate. Ar^+ jet treatment, before gold deposition, and low temperature of substrate, during gold deposition, are found to be factors which favour the post-deposition, thermally induced de-wetting process.

Poster T4-6

Correlation between relevant reaction parameters and properties of magnetite clusters produced by a solvothermal polyol process

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Abstract. Magnetite nanoclusters prepared by a solvothermal polyol process have recently gained widespread interest. Due to their high magnetization while still retaining their superparamagnetic properties as well as high stability in aqueous dispersion they are very useful for growing fields such as catalysis and especially biomedicine. It is possible to tune properties such as cluster and crystallite size by changing some reaction parameters. While these trends have been confirmed and the reactions are very reproducible, when trying to follow literature procedures or scaling the reaction up/down, some of the properties of the magnetite clusters may deviate from the reported ones. Herein, the influence of reaction parameters has been examined that may be responsible for this behaviour. The physico-chemical properties of the magnetite clusters investigated by TEM, FTIR-spectroscopy, XPS, XRD, and magnetization measurements evidence which parameters are important for exactly reproducing results from literature as well as scaling up reactions.

Poster T4-7

Liquid distribution of water and cyclohexane molecules inside carbon aerogels and xerogels under partially saturated conditions

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Abstract. In the present work a comparison between the liquid distribution, under partially saturated conditions inside two carbon aerogel and xerogel samples, was done using the nuclear magnetic resonance relaxometry. The molecules under investigation were water and cyclohexane. They were chosen due to their different interaction with the carbonaceous matrix. It was found a non-uniform coverage of molecules on the pore surface except for the case of cyclohexane filled carbon xerogel when the distribution was uniform. Information about the tortuosity of the two samples was also extracted using pulse field gradient NMR diffusometry. The role of the drying process on pore connectivity and liquid distribution under partially saturated conditions could be monitored.

Poster T4-8

Tissue distribution of intravenous and intraperitoneal administration of SPIONs in a rat model

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Abstract. SuperParamagnetic Iron Oxide Nanoparticles (SPIONs) are used in routine magnetic resonance imaging and some latest technology medical treatments. Still, their effects are not yet fully known or understood. In our study, we analysed the tissue distribution of 50 nm SPIONs in rat organs, blood serum and urine for 24 hours. SPIONs were obtained by the oil mini-emulsion method and clusters were coated with polyethylene glycol (PEG). Rats were injected intraperitoneally or intravenously with SPIONs, and organs were analyzed by histological methods and transmission electron microscopy. Blood serum and urine were analyzed by spectrophotometry. Analyses showed that SPIONs were already in the kidneys and urine at 6 hours post administration with a peak at 12 hours. SPIONs were found also in liver, lungs and spleen mostly at 24 hours' time point. SPIONs were absorbed by the blood stream at as early as 6 hours after administration and were still found in blood 24 hours later. SPIONs have a general distribution in the rat body, with no signs of toxic effects to any of the studied organs. This promotes our 50 nm PEG-coated clusters of SPIONs recipe for an array of medical applications.

Poster T4-9

High quality, nanostructured surfaces fabricated using nanoimprint lithography

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Abstract. Nanoimprint lithography (NIL) is an emerging cost-effective and high throughput lithographic technique, able to pattern low-cost nanostructured surfaces. It relies on the mechanical deformation of a wide range of materials (imprint resists), by using a hard mold with 3D high-resolution nanoscale features. Since its appearance, NIL has been used not only to create nanopatterns, but also to advance the state of the art in the fabrication of nanodevices for electronics, photonics, data and energy storage, and biotechnology. Our work consisted in the perfect transfer of the nanomotifs from the mold on flexible, transparent substrates (polycarbonate – PC, IPS® polymer substrates and poly(methyl methacrylate) – PMMA). The topography and design of the mold was assessed using atomic force microscopy (AFM) technique. For a regular and an accurate replication of the mold, the imprint parameters (temperature, pressure and time) were optimized and each imprinted wafer was assessed using AFM technique.

Poster T4-10

Graphene-gold nanoparticles composites: Synthesis and application

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Abstract. A simple and efficient approach for graphene production, by electrochemical exfoliation of graphite rod in acidic solutions, is reported. The developed method yielded graphene with different oxidation degrees depending on the electrochemical parameters (applied bias, electrolyte concentration). After optimization, gold nanoparticles were chemically attached to graphene sheets. The starting materials were selected taking into account the fact that the presence of the oxygen functional groups positively influences the nucleation and growth of metallic nanoparticles. The obtained nanocomposites were characterized by TEM, SEM, X-ray powder Diffraction, Thermogravimetric analysis and X-ray Photoelectron Spectroscopy and then used to modify a glassy carbon electrode for the electrochemical sensing of hydroquinone.

Poster T4-11

Characterization of Poly (isobutylene - co-maleic acid) sodium salt -cross-linked hydrogel by Low-Field 1D and 2D ^{1}H NMR Laplace Spectroscopy

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Abstract. Superabsorbent hydrogels, cross-linked polymers having the ability to absorb a large amount of water from aqueous medium, can be used, in particular as intelligent materials. Such materials are able to respond to various properties of environmental changes like: solvent composition, pH or temperature. In the same time other aspects of environment like the UV-radiation, during, apriori or aposteriori the formation of hydrogels, can affect the swelling behaviour of hydrogels. The Poly(isobutylene–co-maleic acid) sodium salt-cross-linked was investigated by: i) one-dimensional ^{1}H NMR relaxometry (CPMG pulse sequence), saturation recovery and diffusion methods and ii) two-dimensional T_2–T_2 exchange maps to observe the evolution of dynamic components of hydrogels after hydration. The effects of hydration/dehydration processes, the action of specific environmental factors can be observed by the migration of particular component in the 1D T_2 (T_1) distributions or diagonal and in special extra diagonal peaks in the 2D T_2–T_2 exchange maps. We found that the UV radiation even at less than one hour can affect significantly the swelling properties of polymer hydrogel, probably by destroying the double bonds.

Poster T4-12

Development of erbium doped core-shell Fe_3O_4- $MnFe_2O_4$ magnetic nanoparticles functionalized with polyethylene glycol for magnetic resonance imaging

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Abstract. We report synthesis and characterization of Er doped magnetic nanoparticles with tailored size, shape and chemical composition appropriate for application as new contrast agent for imaging. The magnetic nanoparticles, magnetite Fe_3O_4, manganese ferrite $MnFe_2O_4$ and Fe_3O_4- $MnFe_2O_4$ core-shell type magnetic nanoparticles doped with Er^{3+} were prepared by thermal decomposition method. Biocompatible nanoparticles with good colloidal stability were obtained by coating the as-prepared magnetic nanoparticles with polyethylene glycol (PEG) shell. Physico-chemical characterization (FTIR, TEM, EDX, XPS, magnetic measurements) demonstrate the nanoparticles formation and evidence the effect of rare-earth doping on the structural and magnetic properties of nanoparticles.

Poster T4-13

Smart materials for smart (bio)sensors

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Abstract. Advances in nanotechnology have led to the development of nanoscale biosensors with exquisite sensitivity and versatility as their ultimate goal is to detect any biochemical and biophysical signal associated with a specific disease at the level of a single molecule or cell. The ability to detect disease-associated biomolecules is essential not only for disease diagnosis in the clinical setting, but also for biomedical research involving drug discovery and development. Portable, faster and low-cost devices are highly preferred for replacing time–consuming centralized laboratory analysis. The reduction in sensor size provides great versatility, but the extreme miniaturization while keeping intact the selectivity and sensitivity characteristic to biosensors must be achieved. The sensitivity of biosensors could be increased by using different smart nanomaterials like carbon nanotubes, graphene, nanoparticles while the selectivity is gain when biomolecules are involved (enzymes, antibodies, aptamers). Several examples of nanomaterials involved in the development of biosensors will be presented with a focus on the geometry, miniaturization and multiplexing ability. Tattoo and needle sensors for minimal invasive devices represent the latest approaches in this dynamic field of research.

Poster T4-14

Preparation and functional properties of PVDF-based composites

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Abstract. The demand for high dielectric constant materials and high energy density capacitors has rapidly increased in recent years due to the continuous and rapid development of the electronic industry and the need to store electrostatic energy more efficiently. The combination of dissimilar materials in a composite represents an effective approach for the optimization of the dielectric properties. The addition of ferroelectric (barium titanate, $BaTiO_3$) nanoparticles with high dielectric constant ($k \approx 1000$) enables the relative dielectric constant of the polymer ($k \approx 3\text{-}10$) to be significantly increased without compromising some of the most useful properties of the material. Polymer composites were prepared using polyvinylidene fluoride (PVDF) as a matrix and $BaTiO_3$ nanoparticles (d~100 nm) as inclusions. The composites were fabricated by mixing PVDF and $BaTiO_3$ particles at 200°C using the melt-blend method. The microstructure was observed on fracture surfaces by SEM. The amount of the ferroelectric β phase in the PVDF matrix was determined by FT-IR spectroscopy and the dielectric propeties were determinated at different frequencies and temperature by impedance spectroscopy. Simulation of the field distribution in model composites was performed by 3D finite element modelling.

Poster T4-15

MOF-based catalysts for hydrogen production from formic acid

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Abstract. Formic acid has been recognized as a potential liquid storage medium capable of releasing hydrogen under mild conditions via catalytic decomposition. The hydrogen production from formic acid, using a new type of heterogeneous catalysts based on metallic nanoparticles (MNPs) confined in metal-organic frameworks (MOFs) is presented. The hybrid materials obtained by loading palladium nanoparticles (up to 10%) in UiO-66 were characterized and their catalytic activity and selectivity in formic acid decomposition were investigated.

Poster T4-16

Time-correlated single photon counting of rare-earth doped Ag nanoparticles

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Abstract. Samarium and other trivalent rare earth-doped materials have attracted a great deal of interest lately due to their important role in the development of optical applications such as fluorescent glasses, long-lasting photo-stimulated luminescence, integrated optical photonic devices, optical amplifiers, and biological applications. The fluorescent photosensitive glasses can have applications in photography, fluorescent displays, and computer memories. This study presents the time correlated single photon counting fluorescence investigations of samarium oxide in the presence and absence of Ag colloidal nanoparticles. The degree of fluorescence can be manipulated by combining these two components under controlled irradiation conditions. Time-resolved fluorescence spectroscopy is based on recording the time-dependent intensity profile of the emission signal upon excitation with an ultrashort laser pulse. The presence of the metallic nanoparticles leads to a drastic decrease of the fluorescence lifetimes of Sm due to the interactions of its excited-state with the surface plasmon resonances on the surface of the metal.

Poster T4-17

Structural investigation of polydopamine deposited on silica substrates

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Abstract. Polydopamine (PDA) formed by the oxidation of dopamine is not only a multifunctional biopolymer but also a versatile coating platform for various surfaces. Mussel-inspired adhesives based on dopamine have potential as a universal solution to surface modification by functionalization on hydroxyl and amine group of the PDA coating. The structure and formation of polydopamine is an active area of research. We investigate the structure of polydopamine coated silica nanoparticles by solid state NMR and electron microscopy (SEM/TEM) techniques. Silica nanoparticles were synthesized using ultrasonication by sol-gel process and thin PDA films were coated on these nanoparticles via self-polymerization of dopamine in alkaline condition (10 mM Tris-HCl buffer solution at). ^{1}H, ^{13}C and ^{29}Si NMR spectra were used to study the PDA-silica nanoparticles interface, whereas their morphology was investigated by electron microscopy.

Poster T4-18

Materials based on functionalized poly(benzofurane-*co*-arylacetic acid) for wastewater treatment

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Abstract. Integrated study of both natural water quality and wastewater provides important information regarding the human impact activities in the environmental landscape. Water contamination with heavy metal ions represents a major ecological problem due to their toxic effects on environmental factors and human health. In the last decades, it has been proved that nanomaterials, especially those formed by metal oxides, are effective for the removal of heavy metal ions from wastewater due to their unique structure properties. In order to improve the efficiency of these nanoparticles, they were covered by polymers or functionalized. We report here the functionalization of poly(benzofurane-co-arylacetic acid) with different types of molecules capable to complex heavy metals and their ability to cover magnetic nanoparticles. Such nanomaterials can easily be separated by external magnetic fields and thus offer attractive ways of wastewater treatment. The synthesized polymers and magnetic nanostructures are structural investigated by SEM, TEM, NMR and FTIR.

Poster T4-19

Nanosecond Laser Photo-Induced Heating of Gold Nanoparticles Embedded in a Polymer Matrix - the Influence of Interface Conductance

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Abstract. In the past several years, the interaction between gold nanoparticles and laser light is investigated due to the metal nanoparticles property to generate heat when irradiated with visible light. This phenomenon has important applications in material growth, temperature control distribution, photothermal cancer therapy and drug release. In this work it is modelled, by finite element analysis, the temperature evolution in a nanosecond laser irradiated system that consists of spherical gold nanoparticles embedded in a polymer matrix. Time-dependent evolution of temperature is computed in different points of the system and also the necessary time to reach the thermal equilibrium is investigated. In our analysis, the non-perfect contact between the gold nanoparticles and the surrounding medium is taken into account.

Poster T4-20

Graphene-based Catalysts for Efficient Hydrogen Generation from Formic Acid

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Abstract. Recently, Formic Acid (FA, HCCOH), has attracted considerable attention as a safe and convenient hydrogen storage material due to its high hydrogen content, nontoxicity and excellent stability. FA has been considered a potential liquid storage medium capable to release hydrogen under mild condition via a catalytic decomposition. Despite tremendous efforts, the use of new heterogeneous catalysts with high activity and relatively low cost to replace homogeneous catalysts with difficult synthesis, separating and recycling, remains an important strategy to promote the development of hydrogen generation from formic acid. In this study, we report the hydrogen production from formic acid using an efficient heterogeneous catalyst based on metallic nanoparticles (MNPs) supported on reduced graphene oxide (rGO). The resulted hybrid material was characterized and their catalytic activity and selectivity was investigated.

Poster T4-21

Structural and Magnetic Behaviour of Chemicaly Synthetized $CoPt@Fe_3O_4$ Magnetic Nanoparticles

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Abstract. Ferromagnetic chemically ordered face-centred tetragonal, $L1_0$ CoPt alloy nanoparticles are promising candidates as the next generation of ultrahigh-density data storage media. In order to obtain the exchange coupling between the hard and soft phases the preparation $L1_0$ CoPt nanoparticles with high coercivity, narrow size distribution remains as a challenge. Here we report the fabrication of $CoPt@Fe_3O_4$ exchange coupled nanoparticles by employing as precursors for CoPt phase Co acetylacetonate and Pt acetylacetonate and as reaction media dioctyl ether. In order to obtain a good crystallinity of phases, the as obtained CoPt nanoparticles were annealed at 700 °C in reducing atmosphere ($Ar+10\%H_2$). The soft magnetic phase was obtained by precipitation in basic media of iron salts. The elemental composition of materials was determined by XPS measurements, the structure and microstructure was checked by XRD and TEM analyses. The remanent magnetisation, the coercive field and the exchange coupling between the hard and the soft phases were deduced from magnetic measurements.

Poster T4-22

New electrode materials based on functionalized magnetic nanoparticles for electrochemical application in nitrite detection

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Abstract. We developed new electrode materials based on magnetic nanoparticles functionalized with inorganic shell-like silica, SiO_2 and/or organic shell-like polymers to build up a modified electrode for nitrite detection. Toluidine Blue (TB) was adsorbed on the hybrid systems, like electrochemical mediator and an improvement in stability of the mediator during the electrochemical measurement was observed. Structural and morphological characterization (FTIR, TEM, EDX) demonstrate the hybrid nanoparticles formation and UV-VIS spectroscopy measurement evidence the effect of TB adsorption on the structural and electrochemical properties of nanoparticles. The electrochemical behaviour of modified electrode was investigated by cyclic voltammetry, in order to be used in future as amperometric sensor for nitrites in synthetic and real samples.

Poster T4-23

Plastering mortar with antibacterial and antifungal properties studied by ^{1}H NMR relaxometry

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Abstract. Plastering mortars with good antibacterial (in particular Escherichia coli, Staphylococcus aureus, Enterococcus faecalis, Pseudomonas aeruginosa) and antifungal (Aspergillus niger and Penicillium chrysogenum) properties were studied by 1D NMR relaxometry. Three compositions based on plastering mortar with variable content (5 and 10 %) Ag/ZnO nanopowders and with adequate physical and mechanical characteristics regarding the mechanical strengths (CS IV), good adhesion to the substrate and low water absorption by capillarity (W2) were considered. For a good antibacterial and antifungal effect on mortar surface, concentrations of more than 5 % Ag/ZnO nanopowders (0.05 wt. %) are required. The distributions of transverse relaxation times T_2 were measured at 2 h after preparation (for mortar pasta) and then for the same samples at 2, 7, and 28 days during the hydration of mineralogical components. The T_2 distributions are characterized by four components associated with hydration water and three types of pores of different dimension. The formation of pores hydration process are strongly dependent on the Ag/ZnO nanopowders content but finally at 28 days the pores distributions looks similar.

Poster T4-24

Graphene oxide – metal nanoparticle composites: preparation and characterization

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Abstract. Graphene oxide (GrO), although it has received less attention than its reduced form – graphene – presents some very interesting properties from the adsorption and catalytic point of view. Basically, it has the same few layers hexagonal sp^2 C structure as graphene, but it presents a series of oxygenated functional groups bonded to the carbon structure, such as: carboxyl, carbonyl, hydroxyl, ethoxy etc. For processes involving adsorption these functional groups act like anchors favouring the attachment of foreign molecules to the surface. The deposition of metal nanoparticles (MeNP) on GrO is challenging due to the necessity to preserve the oxygenated nature of the surface, forbidding thus the in-situ reduction of metal precursors, which is the most used method to obtain small and well dispersed MeNP on a solid surface. In this work, the preparation of Pt-GrO will be presented using the deposition of already formed PtNP on GrO. The characterisation techniques (XRD, TGA, TEM) demonstrate that the obtained composite presents a homogenous structure of well dispersed PtNP deposited on GrO (which preserve the original structure as well).

Poster T4-25

Magnetic properties of Fe_3O_4-TiO_2:Eu composite nanoparticles

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Abstract. This work refers to the influence of Eu doping on the magnetic properties separable Fe_3O_4-TiO_2 composite nanoparticles with photocatalytic activity. In this respect, Fe_3O_4-TiO_2:Eu nanocomposites were prepared by seed mediated growth of TiO_2:Eu through a sol-gel method onto preformed magnetite resulted from co-precipitation method. Different Eu concentration precursors were used for doping. Room temperature hysteresis measurements as well as magnetization versus temperature in zero field cooled – field cooled regime indicates that the nanocomposite exhibit superparamagnetic behaviour. The temperature dependence of saturation magnetization and coercive field shows that Eu doping produces a complex magnetic behaviour.

Poster T4-26

Optimization of some heavy metals removal from aqueous solution using biosynthesized magnetite nanoparticles

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Abstract. In the present work, Cd (II), Pb (II) and As (III) removal from aqueous solutions were investigated with magnetite nanoparticles chemically synthesized and obtained using lemon peel extract, as adsorbents in batch experiments. The Box-Behnken experimental design was used to been investigate the effect of some parameters as initial concentration (20-150 mg/L), pH (2-9) and adsorbent dosage (1-5 g/L) on Cd (II), Pb (II) and As (III) removal. Adsorption efficiencies of chemically and biologically obtained magnetite nanoparticles for removal of Cd (II), Pb (II) and As (III) were found to be 18.7%, 59.4%, 17.46% and 46.0%, 98.8%, 48.2%, respectively. The results suggested that the biologically synthesized magnetite nanoparticles may be used as efficient absorbent for removal of Cd(II), Pb(II) and As (III) from aqueous solutions.

Poster T4-27

Growth of Cu_2ZnSnS_4 thin films on Si (100) substrates by PLD

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Abstract. Cu_2ZnSnS_4 is one of the attractive materials used as absorber layer in solar cells because it is estimated that Cu_2ZnSnS_4 has the band gap energy of 1.4-1.5 eV and the absorption coefficient over 10^4 cm^{-1}. This material has the advantages of low price, relatively low toxicity and abundance in the Earth's crust constituent elements. However, the presence of volatile phases such as tin chalcogenide compounds and elementary zinc substance poses an inevitable challenge for growing pure kesterite without spurious phases. The presence of spurious phases can deteriorate the performance of solar cells as reduced open circuit voltage and shorter carrier lifetime. The successful deposition of high- quality CZTS films strongly depends on reliable and optimal fabrication techniques. It is known that through the use of PLD technique, even for complex materials, the stoichiometry of the target is preserved within the deposited film. Thus Cu_2ZnSnS_4-based thin films were grown on Si (100) using PLD technique in different deposition conditions. X-ray diffraction and Raman spectroscopy was used to investigate the influence of the deposition parameters on structural characteristics. The morphology of the obtained thin films was evidenced using SEM microscopy.

Poster T4-28

Green method for the preparation of chitosan / carbon base nanomaterial and its applicability in heavy metal ion detection

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Abstract. Carbon-based materials are currently at the forefront of materials research due to their outstanding physical, mechanical and electrical properties and exceptional catalytic/electrocatalytic activity. The ability to be dispersed in various polymer matrix leads to a new class of polymer nanocomposites with a wide range of applicability (e.g. food packaging, biosensors, water treatment or drug delivery). The main goal of this study was to provide a facile, rapid, inexpensive way for the green, one-step and large-scale preparation of chitosan / carbon base nanomaterial, trough electrochemical exfoliation of graphite rods, without the use of any organic solvent. The obtained nanocomposite was characterized from morphological and structural point of view. Furthermore, the applicability in environmental electroanalysis of chitosan/carbon based-modified electrodes, for accurate detection and quantification of heavy metal ions from aquatic systems, was also reported.

Poster T4-29

Hybrid ZnO/FePc nano-diode fabricated by molecular beam epitaxy

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Abstract. In the last decade, there has been significant development in the areas of nano-electronics. Organic, flexible and transparent electronics based on metal oxide inorganic semiconductors have shown potential for transparent thin film transistors and low cost large area displays. Zinc oxide is considered to be one of the most important materials for transparent electronics, due to its attractive properties such as direct band gap, nontoxicity, and high stability. We have designed and developed a Zinc Oxide and Iron Phthalocyanine based hybrid diode using Al doped ZnO as transparent conducting electrode on two types of substrates: microscope glass and polycarbonate (flexible substrate). The current-voltage characteristic certifies the quality of the obtained diodes. The V-I measurements give a maximum value of 0.15mA/cm^2 at 2V in the current density in the case of the junction fabricated on flexible substrate with small built-in potential (Vbi <1V). The high transmission of AlZnO electrodes (T > 80%) as well as the diode fabrication on polycarbonate substrate offer the opportunity to use these diodes in transparent and flexible electronics.

Poster T4-30

Ni@MOF catalysts for low temperature CO_2 methanation

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Abstract. Methanation of CO_2 by hydrogen has gained lately renewed scientific and technological interest due to both environmental (fixation of CO_2) and energetic (chemical storage of H_2 in methane) advantages. Considering that CO_2 methanation is a highly exothermic reaction, low temperature working catalysts are highly desired for an efficient process. This goal may be reached by enhanced activation of the reactants, which could be achieved by employment of supported catalysts with large dispersion of the active metal species (H_2), and by use of high adsorptive supports (CO_2). In this context, MOFs are a viable alternative due to (1) their very large surface areas which can favour a high dispersion of the metallic active sites, as well as (2) due to their special porous structure which can serve as trap for the activation of CO_2. We report on the use of Ni(10wt.%)@MOF (UiO-66, MIL-101) as catalysts in the methanation of CO_2 at temperatures below 350°C. Catalysts prepared by the classical impregnation method or the 'double solvent' method showed promising performance in the methanation process (CO_2 conversion values up to 60% and CH_4 selectivity values up to 85%). The employed characterization techniques revealed a good dispersion of the metallic nanoparticles (XRD, TEM) on/in the MOF support, as well as a consistent chemisorption capacity for both H_2 and CO_2 (H_2-TPD and CO_2-TPD).

Poster T4-31

Synthesis, characterization and efficiency of PSF/MCM-41 membranes for CO_2 removal

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Abstract. The CO_2 removal from flue gases using unconventional techniques based on membranes, known a significant interest in industry. Mixed matrix membranes combine the advantages of organic (easily processable and low cost) and inorganic phases (high selectivity, mechanical resistance, chemical and thermal stability). In this study, polysulfone incorporated with mesoporous inorganic materials MCM-41 were proposed. MCM-41 with 1160.878 m2g-1 specific surface area and 3.8 nm pore size were obtained and used as inorganic filler. The mixed matrix membranes were prepared by casting method. The effects of MCM-41 loading (5-20 wt.%) on the membrane characteristics were studied using SEM, XRD, TGA, while the gas transport properties were investigated using pure gas permeability tests of CO_2 and CH_4 and also gas mixtures permeation tests of 10vol%CO2/90vol%N_2. The TGA analysis confirmed that the membranes are appropriate for operating at high-temperature condition, the complete degradation of polymeric chain being achieved after 650°C. Well dispersion of MCM-41 particles in the polymer matrix was observed for 10 wt.% of MCM-41 into PSF membrane, in comparison with 20 wt.% of MCM-41 in PSF membrane where particles agglomerations were visible in SEM images. Even if the inorganic particles adhered each other the obtained membranes PSF/20 wt.% presented an ideal selectivity up to 41.52 and a real selectivity up to 45.06 for CO_2/N_2.

Poster T4-32

Plaster mortars with polymer fibers and additives investigated by ^{1}H NMR relaxometry

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Abstract. Plaster mortars with polypropylene (*pp*) fibers and/or additives were investigated by ^{1}H NMR relaxometry. Two recipes are proposed and are based on a commercially available sample or are self-prepared and have different content of polypropylene fibers, which play the role of reinforcement agent, and/or Sika additive which is a waterproofing agent. The distributions of transverse relaxation times, T_2 were obtained at 1, 3, 7 and 28 days after preparation. For the majority of T_2-distributions four peaks are observed and are associated with the hydration water (to the mineralogical components) and water in small, medium and large pores. The evolution in time, from 1 to 28 days, of the T_2-distributions indicates the effects of *pp* fibers and Sika additive in the formation of pore microstructure. The degree of homogeneity of prepared receipts was evaluated from the relative peak-width and compared with mechanic measurements. Finally, we shown that the inverse of the transverse relaxation time values, T_2^{-1}, characteristic to the hydration water depends linearly on the resistance at compression measured for the 1-28 days period, proving the important role of hydrations to the mechanic properties of the final product.

Poster T4-33

FT-IR and morphological (SEM) investigation of starch based composite reinforced with miscanthus fibers

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Abstract. The properties and structure of starch based materials can be improved by reinforcement with natural fibers due to the chemical similarity of vegetal fiber and starch. In this study, natural fiber reinforced starch based composites have been developed by extrusion procedure. The reinforcement materials used are miscanthus fibers in minced form. A set of 5 formulas of composite material with various fiber ratios (up to 20%) were prepared and investigated. FT-IR spectroscopy supported the molecular interactions due to the reinforcement with miscanthus fiber of starch-based composite. The morphological study of the fractured surface has been done using scanning electron microscopy (SEM), and suggested sufficient homogeneous dispersion and randomly orientation of fibers within the starch-based matrix and good interfacial adherence between matrix and fibers.

Poster T4-34

Platinum mesoporous silica catalysts for liquid media oxidation

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Abstract. The mesoporous silica was successfully used as the support to immobilize transitional metals such as platinum, both in physical and chemical methods. UV-VIS, FT-IR, XPS, EXAFS and N_2 adsorption were applied to characterizing the obtained catalysts. The results of some liquid media oxidation (such as unsaturated alcohols or cyclohexene) revealed that the supported catalysts have higher catalytic activity as their homogenous counterpart does.

Poster T4-35

The efficiency of the multi-walled carbon nanotubes used for the antibiotics removal from wastewaters generated by animal farms

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Abstract. The present paper describes the efficiency of several types of multi-walled carbon nanotubes (MWCNTs) for the retention of 14 antibiotics (ampicillin, ceftazidime, cefepime, imipenem, piperacillin, tazobactam, tetracycline, erythromycin, ciprofloxacin, norfloxacin, vancomycin, gentamicin, sulfamethoxazole, and thrimetoprim) from aqueous solutions. The functionalized MWCNTs were characterized by Fourier transform infrared spectroscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Also, different surfactants were used for a better dispersion of the MWCNTs in the aqueous solutions, in order to increase their contact surface with the antibiotics. The antibiotics retention was evaluated by quantitative assessment using high performance liquid chromatography coupled with the diode array, fluorescence, and mass spectrometer detectors (HPLC-DAD/FD/MS), after the solid phase extraction (SPE) with Oasis HLB cartridges. The retention percentages of the selected antibiotics from waters ranged between 40-97%, with the exception of sulfamethoxazole (5.48%) and trimethoprim (0.00%). The best retention percentages were obtained for norfloxacin (97.03%) and ciprofloxacin (97.10%). Removal of antibiotics from wastewaters using nanotechnology, in order to reduce their negative effects and antibiotic resistance, represents a promising tool in the future wastewaters treatment.

Poster T4-36

New properties of Fe_3O_4@SnO_2 core shell nanoparticles following interface charge/spin transfer

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Abstract. The synthesis and properties of Fe_3O_4@SnO_2 core-shell nanoparticles are reported in the present paper. To form Fe_3O_4@SnO_2 nanocomposites (FeSn-Ox), the magnetite (Fe_3O_4) nanoparticles were covered with SnO_2 semiconductor through the use of the seeding method followed by a thermal treatment. XRD studies reveal that the synthesized composite nanoparticles contain mainly Fe_3O_4 and SnO_2 in different proportions depending on the preparation conditions. The composition of nanoparticles and their core-shell architecture were evidenced by XPS and confirmed by Fourier analysis of HRTEM images. Magnetic studies also indicated that FeSn-Ox samples exhibit superparamagnetic behaviour at room temperature. It was found that the SnO_2 shell nanocrystals contain ordered magnetic moments formed through a charge/spin transfer process across the interface (carrier-mediated ferromagnetism). The analysis of UV-Vis and photoluminescence (PL) spectra of FeSn-Ox composites also show position modifications of SnO_2 impurity band gap levels in accordance with the charge/spin transfer between Fe_3O_4 and SnO_2 outer shell.

Poster T4-37

Magnetic nanoclusters doped with rare earths metals

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Abstract. In the field of multimodal imagistic, magnetite and rare earth metals provide interesting properties. We present the synthesis of new materials based on magnetic nanoclusters (MNC) doped with rare earth metals by one step synthesis procedure using solvothermal method**.** The obtained clusters possess high saturation magnetization up to 40 emu/g and uniform spherical shape evidenced by transmission electron microscopy. Energy-dispersive X-ray microanalysis and X-ray photoelectron spectroscopy (XPS) confirmed the elemental composition of the samples. X-ray diffraction analysis proved the homogeneous distribution of the trivalent rare earth ions in the inverse-spinel structure of magnetite and the increase of crystal strain upon doping the samples. XPS study reveals the valence state and the cation distribution on the octahedral and tetrahedral sites of the analysed samples. The observed shift of the XPS valence band spectra maximum of the MNC in the direction of higher binding energies after rare earth doping and theoretically valence band calculations proves the presence of rare earth metals in octahedral sites.

Poster T4-38

Electrochemical detection of phenolic compounds with graphene-porphyrin modified electrode

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Abstract. Phenols of anthropogenic origin exist in the environment due to the activity of various industies (chemical, pharmaceutical or petrolier). Recent studies have shown that the exposure to catechol (CAT) induces various diseases, such as high-blood pressure, kidney damage or, in high-doses, even convulsions. Due to its high toxicity and harmful effects on human health, catechol detection has become of great importance. This work presents a novel approach for the synthesis of graphene nanosheets through electrochemical exfoliation of graphite in the presence of 5,10,15,20-tetra(4-pyridyl)porphyrin (TPyP), in 0.2 M KCl electrolyte. The performances of the electrochemically exfoliated graphene (EGr) attached to the glassy carbon (GC) surface were evaluated. It was found that the CAT redox process was highly accelerated when EGr-modified GC electrode was used. In addition, the peak currents were significantly higher than those obtained with bare GC substrate. As expected, the GC electrode has low sensitivity towards CAT (6 mA/M), a narrow linear range (10^{-5} - 10^{-4} M) and a high detection limit (LOD = 1.42 x 10^{-5} M). In contrast, the EGr/GC electrode has a higher sensitivity (245 mA/M), a considerably wider liner range (10^{-6} - 10^{-4} M) and lower detection limit (LOD = 2.5 x 10^{-6} M).

Poster T4-39

New germanate system with paramagnetic ions

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Abstract. Nowadays there is a great interest for new materials with properties appropriate for medical applications. The aim of this study was to find a new system with possible applications in medicine and having no adverse effects in human body. As it is known, zinc and germanium (at low content) show antibacterial properties. Paramagnetic ions are usually used as contrast agent in magnetic resonance imaging. Therefore, new zinc oxide – germanate systems doped with different paramagnetic ions were prepared and studied by XRD, FT-IR spectroscopy and magnetic susceptibility measurements. The FT-IR data permitted to follow the compositional evolution of the structural units that build up these materials, namely the structural changes determined by increasing the doping with paramagnetic ions. Magnetic susceptibility data offer information concerning the evolution of the magnetic behaviour of the studied systems as function of their paramagnetic ions content.

Poster T4-40

Photocatalytic performance of magnetic composites based on Fe_3O_4 and Gd doped TiO_2

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Abstract. Photocatalytic degradation using semiconductors has been found to be a highly effective method for waste water treatment. The advantages of this method are its potential to complete mineralization of pollutants and the use of non-toxic, cost effective catalysts. Among the studied semiconductors, TiO_2 shows high photocatalytic degradation performance against organic dyes. In the present work, we report the experimental results obtained on photodegradation of RhB using Gd doped TiO_2 /Fe_3O_4 composites. By using Gd as a dopant we try to extend the spectral response of TiO_2 into the visible region while the presence of Fe_3O_4 compound may solve the problem of photocatalyst recovery**.** The XRD measurement shows the specific peaks corresponding to magnetite (Fe_3O_4) and anatase (TiO_2) phases. A secondary phase of $FeTiO_3$ has been evidenced. The morphologies and sizes of nanoparticles were characterized using transmission electron microscopy. The best photodegradation rate was obtained for a doping content of 0.5% Gd. The photocatalyst presents a good stability after four cycles. The photodegradation pathway is also highlighted.

Poster T4-41

Structural analysis of Sb_2O_3 doped lead-lead dioxide glass ceramics by XRD and XAS spectroscopy

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Abstract. Batteries are essential in modern society to sustain our high tech lifestyles. As an excellent source of mobile energy, batteries are receiving a large amount of attention compared to other available products. For spent battery, the positive and negative electrode active materials are composed of $PbO_2/PbSO_4$ and $Pb/PbSO_4$ and lead is the most important raw material of lead acid batteries. A new vitreous system based on metallic lead and lead dioxide doped with antimony trioxide was prepared by melt quenching method. As starting materials were used active electrodes of the spent battery mixed in suitable proportion $Pb:PbO_2$=1:9, 2:8, 3:7, 4:6, 5:5, 6:4, 7:3, 8:2, 9:1 with 10mol% Sb_2O_3. Structural and behavioral investigation of samples was performed by X-ray Diffraction (XRD) analysis and XAS spectroscopy. XRD patterns permits the identification of two separated phase: a metallic phase consists of metallic Pb and PbO crystalline phases and the vitroceramic one with different oxidic and sulphate crystalline phases of the lead ions. Extended X-ray absorption fine structure (EXAFS) is a specific element of the scattering technique in which a core electron ejected by an X-ray photon probes the local environment of the absorbing atom.

Poster T4-42

Behaviour of zirconia-magnesia ceramics in the presence of iron (III) oxide

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Abstract. ZrO_2-MgO ceramics were attracted a great deal of interest recently due to their excellent properties and for widely industrial applications like sensors, refractory materials, biomaterials and fuel cells. Many challenges were done for optimization of synthesis methods of these ceramics. The aim of this work was to explore the structure of the ceramic system with the $xFe_2O_3 \cdot (100\text{-}x)[ZrO_2 \cdot MgO]$ composition where x=0-40mol% Fe_2O_3. MgO has role of stable agent of the cubic ZrO_2 phase while Fe_2O_3 act as both stable agent and activating agent due to its lower melt temperature. Obtained samples were characterized by investigations of XRD, FTIR, UV-Vis and EPR spectroscopy and density measurements.

Poster T4-43

Synthesis and characterization of Fe_3O_4@SiO_2 core-shell nanoparticles functionalized with vinylimidazole-rare earth complexes

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Abstract. In search for magnetic nanoparticles with multifunctional complementary characteristics in this study, magnetite nanoparticles functionalized with vinylimidazole-rare earth complexes were analyzed. The shape, size and structure of the obtained samples were determined by X-ray diffraction and transmission electron microscopy. Electron energy loss spectroscopy and X-ray photoelectron spectroscopy (XPS) analysis showed that the obtained nanoparticles comprise a crystalline magnetite core and a silica shell bearing on the outer surface functional groups of vinylimidazole. The presence of rare earth ions on the sample surface was proven by XPS. The magnetic properties of the nanoparticles were investigated using a vibrating sample magnetometer. It was found that the rare earth doped magnetite nanoparticles were superparamagnetic with high saturation magnetization.

Poster T4-44

Photocatalytic degradation of amaranth dye using PVC/TiO_2-Ag/graphene films under natural daylight exposure

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Abstract. Photocatalysis is already recognized as green and viable strategy for environmental problems, such as water pollution with various hazardous chemicals. Poly(vinyl chloride) (PVC), titanium dioxide (TiO_2)-silver (Ag) nanocomposite and graphene oxide as starting materials were used to obtain photocatalytic films for amaranth azo dye degradation from water. The TiO_2-Ag nanocomposites with Ag:Ti molar ratio of 0.025 were prepared based on a combined chemical/thermal procedure. Graphene oxide was obtained from natural graphite using an improved Hummer's method. A comparative photocatalytic activity of films with different PVC concentrations (25 or 50 mg/sample) containing the same amount of TiO_2-Ag and TiO_2-Ag/graphene on the amaranth photo-degradation was investigated. The experiments were performed in a cloudy day with low temperature (4.8°C) and increased humidity (88%) from December (Cluj-Napoca, Romania). Significant degradation efficiencies (between 62.4 and 79.1 %) of films after two hours of daylight exposure in amaranth solutions ($2x10^{-5}$ M) were demonstrated. The photocatalytic performance of as-prepared materials on amaranth degradation indicates that they could be promising candidates for other azo dyes removal from aqueous solutions using an eco-friendly and cost-effective source: natural daylight.

Poster T4-45

Preparation of MnO_2 nanocatalyst used for biofuel production

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Abstract. The MnO_2 nanoparticles, used as catalyst, determine an enhanced reaction rate of the transesterifications process thus being very attractive for biodiesel production. The aim of the present research was to prepare MnO_2 nanoparticles by chemically and biochemically (using plant extracts) procedures. The biochemically synthesis was performed by sonochemical method using extracts from three different plants: rosemary, oregano and tarragon. The comparison of the results revealed that the samples prepared using plant extracts show smaller sizes, surface specific area and porosity much higher than in case of chemically prepared sample. Among them the MnO_2 nanoparticles obtained by the use of tarragon extracts were further tested for microwave assisted transesterification studies. The prepared nanoparticles were tested as catalyst in microwave-assisted transesterification of grapes residues and seeds oil. The results were compared with those obtained with yeast (*Saccharomyces cerevisiae)* for biofuel obtaining. The best results were obtained with MnO_2 prepared with oregano extract.

Poster T4-46

Chitosan coating of green synthesized magnetite nanoparticles: preparation and characterization

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Abstract. Among the different magnetic materials, magnetite (Fe_3O_4) has been intensively studied due to its unique magnetic and electric properties and its applications in medical diagnosis and therapy, targeted drug delivery, magnetic resonance imaging and cancer hyperthermia treatment, as nanosorbent for environmental remediation, etc. Consequently, the development of facile and green methods for synthesizing magnetite nanoparticles (Fe_3O_4 NPs) is an issue of interest and still a challenge for materials scientists. Some of these synthesis trials involve the use of various plant or fruit extracts as surfactants. The present contribution reports a green synthesis method of Fe_3O_4 NPs using agro-waste extracts obtained from *Persea americana* (avocado) and *Citrullus lanatus* (watermelon), and their further coating with the natural polymer chitosan. The as-prepared magnetic samples were characterized by different techniques including X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Brunauer-Emmett-Teller method (BET), X-ray photoelectron spectroscopy (XPS), and vibrating sample magnetometry (VSM). For comparative reasons, bare and chitosan-coated Fe_3O_4 NPs were also prepared by traditional chemical procedure.

Poster T4-47

Morphologic and structural characterization of magnetic recoverable Fe_3O_4/SnO_2 photocatalyst

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Abstract. In recent years, novel nanotechnologies have allowed great improvements in the synthesis of photocatalysts with well-controlled size, shape and surface properties. Semiconducting metal-oxide materials such as TiO_2, ZnO and SnO_2, being environmentally friendly materials, are very interesting when used as photocatalysts especially for waste water treatment. By combining the properties of both Fe_3O_4 and SnO_2 into binary oxide composite nanostructures would greatly broaden their application areas ranging from photocatalysis to materials for Li-ion batteries (LIBs) or for magnetic resonance imaging (MRI). Composite Fe_3O_4/SnO_2 nanoparticles were realized by deposition of SnO_2 nanoparticles onto the surface of previously prepared Fe_3O_4 nanoparticles. The method used for preparation of SnO_2 nanoparticles was the chemical precipitation. X-ray diffraction (XRD), transmission electron microscopy (TEM) and high resolution (HRTEM), magnetic, surface area and porosity measurements reveal that as-prepared composite nanospheres exhibit, besides magnetic properties, a well-defined structure, uniform sizes, high surface areas and large pore volumes. Finally, it was shown that Fe_3O_4/SnO_2 magnetic composite nanoparticles exhibit good photocatalytic activity toward the degradation of RhB solution thus making them suitable as an efficient recoverable photocatalyst.

Poster T4-48

Functionalization of iron/platinum nanoparticles with core-shell structure

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Abstract. Two types of $Fe@FePt_{aTT}@P3HT$ nanoparticles (FFP/P3HT) and $Fe@FePt_{aTT}@SiO_2@NH_2$ ($FFP/SiO_2/NH_2$) were prepared to use for molecular magnetic separation and capture from water based solutions. The two types of nanoparticles were tested for the capture of amino acids (lysine, cysteine, alanine in different concentrations) from aqueous solutions and also for their magnetic separation. The retention of amino acids on the surface of the nanoparticles was proved by using high performance liquid chromatography. It was found that the best yield of alanine and cysteine retention was obtained with 40 mass ratio between nanoparticles : amino acids. Alanine was best retained on $Fe@FePt_{aTT}@P3HT$ after 4 hours (54% retention rate), cysteine and cystine were best retained on $Fe@FePt_{aTT}@SiO_2@NH_2$ (60% retention rate). Lysine was best retained on $Fe@FePtaTT@SiO_2@NH_2$ after 4 hours (65% retention rate) with nanoparticles : amino acids mass ratio = 10.

Poster T4-49

Simultaneously imaging of the thermal diffusivity and effective infrared absorption coefficient of GaAs wafer using lock-in thermography

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Abstract. In this work, we report on simultaneously imaging of the thermal diffusivity and effective infrared absorption coefficient of GaAs wafer using infrared lock-in thermography. The phase images were extracted from the temperature modulation of the investigated surface at different excitation frequencies, by applying the lock-in detection for each pixel of the recorded image. The resulting images were analyzed using the thermal wave model in the transmission configuration. The thermal diffusivity and effective infrared absorption coefficient were estimated from the best fit of the theoretical model to the experimental data applied for each pixels of the phase images. Finally, pre-processing methods, using different filters, were applied in order to enhance the quality of the images. The results demonstrate that the LIT technique in transmission configuration provides spatial information about both the (effective) infrared absorption coefficient and thermal diffusivity of semiconductor crystals.

Poster T4-50

Yttria and sodium oxide stabilized silica-zirconia ceramics for dental applications

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Abstract. The aim of this study was to characterize the formation of the high temperature ZrO_2 crystalline phase in the ceramic system with the $5Na_2O{\cdot}10SiO_2{\cdot}xY_2O_3{\cdot}(85\text{-}x)ZrO_2$ composition where x = 5, 10 and 15mol% Y_2O_3. The obtained samples at 1400°C were characterized by using investigations of X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM) analysis, density measurements, Raman and UV-Vis spectroscopy. The Warren - Averbach X-ray profile Fourier analysis of the (111), (311), (222), (400) and (420) $ZrO_{1.86}$ peak profiles were processed by the XRLINE computer program in order to determine the effective crystallite mean size (D_{eff}). The stabilization of the cubic $ZrO_{1.86}$ crystalline phase depends on the content of yttrium trioxide. The optical band gap values decrease with increasing the Y_2O_3 percentage. These compositional evolutions can be explained considering that with increasing of Y_2O_3 concentration, the excess of yttrium ions leads to the breakdown of $[SiO_4]$ structural units, resulting non-bridging oxygen ions, in agreement with Raman data and hence reduce gap energy. The SEM images of the samples reveal the presence of aggregations having cuboidal shapes. By increasing of Y_2O_3 content in the host matrix, the homogeneity and the crystal density are more highly.

Poster T4-51

Synthesis and characterization of $CuInS_2$-ZnO nanocomposite

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Abstract. The ternary I-III-VI_2 semiconductors are one of the most important candidates for photovoltaic application to ensure largescale application because of their excellent optical and electrical properties. Among these materials, $CuInS_2$ (CIS) has great potential for photovoltaic applications due to its high absorption coefficient of more than 10^4 cm^{-1} and optimum band gap of 1.5 eV. In a traditional inorganic solar cell, photons are absorbed in the p-type CIS layer and converted into electron-hole pairs. The holes are transported through the CIS layer to a back-contact, while the electrons move to the p-n junction where they are transferred to a n-type semiconductor window layer (ZnO, TiO_2, etc). In the present case, we chose to use as window layer nanostructured ZnO. The influence of ZnO content on structural and morphological characteristics as well as onto optical properties of CIS is investigated. The structure, morphology and composition are evaluated using X-ray diffraction and Raman spectroscopy, SEM and TEM microscopy, EDX and XPS. Also, UV–Vis analyses are carried out to assess the band gap value.

Poster T4-52

Dopamine Adsorption on Graphene-based Composite: Electrochemical and Raman Spectroscopic Investigations

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Abstract. Bimetallic nanoparticles (PtNPs:AuNPs 1:2) supported on graphene were prepared by radio frequency chemical vapour deposition (RF-cCVD) method. This composite was used to investigate the adsorption of dopamine and also, to make the electrode for dopamine detection. Thus, a **n**ovel electrochemical sensor based on graphene decorated with bimetallic nanoparticles for dopamine detection was developed (GC/GrPtAu). A series of electrochemical studies for dopamine detection in the absence and presence of interferences were made. For the adsorption studies, the graphene-based composite was treated at room temperature with various concentrations of dopamine/interferences. After a specific protocol, the composite was added to the graphene-based electrode (GC/GrPtAu) and studied by the electrochemical and Raman methods. Using the calibration data obtained from dopamine detection studies, the quantity of dopamine adsorbed on graphene-based composite in normal conditions was determined. Moreover, taking into consideration the Raman measurements of the electrodes (before and after the electrochemical treatment), useful data about the dopamine oxidation products were obtained.

Poster T4-53

Evaluating the lead affinity of V_2O_5 additives used in spent lead acid battery recycling

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Abstract. The need for recycling batteries using environmentally friendly, low cost and low energy consumption methods remains a problem of the modern world. The novel of the eco-innovative and environmental-friendly method of recycling of the active electrodes from spent lead-acid bateries by melt quenching method was proposed for the first time by S Rada et al. The main objective of the present work was to provide a study on structure of the vitreous system with the $xV_2O_5 \cdot (100-x)[4PbO_2 \cdot Pb]$ composition where x=0-20% V_2O_5 in order to integrate the recycled samples as new electrodes for rechargeable batteries. The anodic (Pb) and cathodic (PbO_2) electrodes originated by a spent lead acid battery and V_2O_5 powder in suitable proportions were used as starting materials. A second objective was to understand the electronic conduction mechanism based on the electron hopping between the multivalent states of the vanadium ions. The effect of V_2O_5 concentration on the obtained samples was investigated by X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM) analysis, Fourier Transform Infrared (FTIR), Photoluminescence (PL) and Electron Paramagnetic Resonance (EPR) spectroscopy. XRD patterns permit the identification of the metallic lead phase and of the vitroceramic one with different oxide crystalline phases of the lead ions.

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