12th International Conference

PROCESSES IN ISOTOPES AND MOLECULES

Cluj-Napoca 2019

Organizing Committee INCDTIM

Adrian Bot - *president*
Claudiu Filip
Gabriel Popeneciu
Diana Nicoara
Ioan Turcu
Emanoil Surducan

Secretariat

Adriana Vulcu
Diana Lazar
Ioana Feher
Alia Colnita
Oana Onija
Izabella Szabo
Dan Zotoiu

Scientific Committee

Carlo Altucci	Naples University "Federico II" Italy
Vasile Chis	Babes-Bolyai University, Faculty of Physics, Cluj-Napoca, Romania
Mihai Gligan	National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
Yongho Hur	Green Energy Institute, Mokpo, Jeollanam-do, South Korea
Changheon Kim	Green Energy Institute, Mokpo, Jeollanam-do, South Korea
Cheng Yu Lai	Florida International University, Miami, USA
Renata de Lima	LABiTON - Laboratório de Avaliação de Bioatividade e Toxicologia de Nanomateriais, Sorocaba University, Sorocaba-SP, Brazil
Alina Magdas	National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
Peter V. Mercea	Fabes Research, Germany
Jun Onoe	Nagoya University, Japan
Denisa Stet	Technical University of Cluj-Napoca, Faculty of Electrical Engineering
Ovidiu Pana	National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
Valer Tosa	National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
Mihai Varlam	National Institute for Research and Development of Cryogenic and Isotopic Technologies – ICSI Rm. Valcea, RO
Agnes Vibok	University of Debrecen, Faculty of Natural Science, Hungary
Nicolae Zamfir	Horia Hulubei National Institute for Research and Development in Physics and Nuclear Engineering, Bucharest Romania
Peter Zavodszky	Institute of Enzymology, Hungarian Academy of Sciences Budapest, Hungary

Welcome at PIM 2019

It is a pleasure of the National Institute for Research and Development of Isotopic and Molecular Technologies to host the 12th 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 2019 provides a stimulating 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. The micro-symposium: *New Trends in Alternative Energies* is scheduled in the last day, in parallel with the regular scientific sessions. This will be entirely devoted to strengthening the collaboration relationships with the Green Energy Institute, Mokpo, Jeoallanam-Do province, South Korea.

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

Micro-symposium – New Trends in Alternative Energies

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

Different approaches to understand the interactions between biomolecules

C Altucci[1,2], **L Altucci**[3], **F Bajardi**[1,2], **R Benedetti**[3], **S Capozziello**[1,2,4], **M R Del Sorbo**[5], **A Nebbioso**[3], **M Singh**[1], **H G Stunnenberg**[6] **andM Valadan**[1,2]

[1] Dipartimento di Fisica "Ettore Pancini", Università degli Studi di Napoli "Federico II", Via Cintia, I-80126 Napoli, Italy

[2] Istituto Nazionale di Fisica Nucleare (INFN), Sez. di Napoli, Via Cintia I-80126 Napoli, Italy

[3] Dipartimento di Biochimica, Biofisica e Patologia Generale, Università degli Studi della Campania "L. Vanvitelli", Vico L. De Crecchio 7, I-80138 Napoli, Italy

[4] Gran Sasso Science Institute, Via F. Crispi 7, I-67100 L'Aquila, Italy

[5] Istituto Statale d'Istruzione Superiore "Leonardo Da Vinci", Via F. Turati 10 I-80040 Poggiomarino (NA), Italy

[6] Department of Molecular Biology, NCMLS, Radboud University, 6500 Nijmegen, the Netherlands

E-mail: carlo.altucci@unina.it

Abstract. The current bottleneck in probing interactions between biomolecules, such as DNA-protein interactions, is often caused by the fact that chemical crosslinkers, used to fix interaction partners, do not discriminate direct and indirect bindings or short-lived chromatin occupancy. We describe a novel application of UV laser-induced (L-) crosslinking and demonstrate that a combination of chemical and L-crosslinking is able to distinguish between direct and indirect. The combination of chemical and L-crosslinking offers an exciting andunprecedented tool for biomedical applications, where the attention is focused to analyse or re-visit DNA and RNA sequences and their possible molecular configurations while interactions take place. Based on methods derived from Chern-Simon super-gravity adapted to describe interactions between nucleic acids, we analyze the KRAS human gene sequence and its mutations. Interestingly, our model is capable to identify and possibly predict the position of mutations within a sequence. The selected sequence and its mutations are also analyzed by means of Information Entropy methods to corroborate our results.

Plenary Pl-2

Improved analytical sensitivity of photothermal lens technique using novel optical methods

H Cabrera[1,2]

[1] National Institute for Nuclear Physics, 99 Padriciano, 34149 Trieste, Italy

[2] The Abdus Salam International Centre for Theoretical Physics, 11 Strada Costiera, 34151 Trieste, Italy

E-mail: hcabrera@ictp.it

Abstract. We present new ways of improving the sensitivity of the photothermal lens technique by using two different approaches: a multi-pass probe beam configuration and a pump-probe photothermal scheme based on the self-mixing effect. As a result of multiple passes of the probe beam through the sample, the first method dramatically increases the sample path length enabling highly sensitivity measurements using very low excitation power. The absorption spectra and high absorption overtones of ethanol and water, as well as, ng/L metals concentrations weremeasured. In the second approach the probe beam is re-injected in the laser cavity, thus the same laser is simultaneously acting as a probe and detector enabling a compact configuration for sensing. In addition, the sensitivity of the method is highly improved because the signal is amplified within a Fabry-Perot cavity which is very sensitive to the optical re-injection therefore requiring small volume of liquid for testing.

Plenary Pl-3

Quality and safety of healthy meat products: biogenic amines

C Ruiz-Capillas[1] **and A M Herrero**[3]

[1] Institute of Food Science, Technology and Nutrition (ICTAN-CSIC), Madrid, Spain

E-mail: claudia@ictan.csic.es

Abstract. Food safety and quality are some of the main concerns of consumers and health agencies around the world (EFSA, WHO, etc.). Over the last few years, the link between human health and nutrition has been strongly established and healthiness has increasingly become a quality criterion in consumers choice of any type food. Based on this, nowadays there exist new tends in the design of healthy food, particularly in meat products, which are important components of the diet in developed countries. In this sense, there is currently work in progress on the development of meat derivates with specific characteristics aimed to influence and improve some body functions whilst still providing basic nutrition needs. However, these new forms of processing could induce or alter de formation of some potential toxic compounds such as biogenic amines. The presence of these amines in food is of interest for two reasons: firstly, for toxicological reasons, in the sense that high levels of dietary biogenic amines can be toxic for certain consumers, and secondly, for their role as possible quality indicators of the products. The formation and control of biogenic amines in these new products need a deeper understanding to ensure their high levels of quality and safety.

Plenary Pl-4

Filtering molecules with electrostatic

I Bodrenko[1]**, S. Milenkovic**[3]**, S Acosta-Gutierrez**[2] **and M Ceccarelli**[1,3]

[1] Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali, Unita di Cagliari, Cagliari, Italy

[2] Department of Chemistry, University Central London, United Kingdom

[3] Dipartimento di Fisica, Universita di Cagliari, Cagliari, Italy

E-mail: matteo.ceccarelli@dsf.unica.it

Abstract. In this talk I'll summarize the effort of our group to combine numerical simulations and electrophysiology with a multi-scale approach for quantifying the passive transport of small molecules through membrane proteins. Starting from some general bacterial pores used as model systems we identified the way in which molecules are selectively transferred in and out from bacteria. The two structural features controlling transport are (i) the hourglass shape of the pore, and (ii) a segregation of charges in the central region. The former property avoids the uncontrolled flux of molecules, creating an unselective barrier for penetration. The latter on the other hand can be very specific: by creating a transversal electric field, it allows molecules with a particular dipole moment to have high flux. This mechanism, an entropic general barrier compensated by specific electrostatic properties, has the advantage to avoid saturation. Further these structural features can be easily transferred in designing synthetic nanopores for selecting/sensing specific molecules.

Plenary Pl-5

Label-free analysis of biomolecules: enzyme vs. nanozyme-based sensors

M Florescu and M David

Transilvania University of Brasov, Faculty of Medicine, Eroilor Str. 29, 500036, Brasov, Romania

E-mail: florescum@unitbv.ro

Abstract. Biomolecular analysis is very important in various fields of application, such as clinical diagnosis, food analysis, environmental monitoring and pharmaceutical development. Employing biomolecules, like enzymes, as analytical tools, offer big advantages for real-time analysis due to their high specificity, selectivity and quick response. For this purpose, the enzyme should be immobilized on different surfaces where the immobilisation process can modify enzyme specific conformation and access of substrate to its active site. Nanozymes are nanomaterials with enzyme-like characteristics and they address the limitations of natural enzymes and conventional artificial enzymes.

In this talk, biomolecular analysis using natural enzyme-based biosensors versus nanozyme-modified sensors are evaluated and discussed. Thus, it summarizes different strategies for both enzyme immobilisation on biosensor surfaces and modulation of activity and selectivity of nanozymes together with the corresponding catalytic mechanisms and analytic parameters for biomedical and food applications. **Acknowledgments***:* This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0062, contract no. 58, within PNCDI III. We hereby acknowledge the structural founds project PRO-DD (POS-CCE, O.2.2.1., ID 123, SMIS 2637, No 11/2009) for providing the infrastructure used in this work.

Plenary Pl-6

Post-photosynthetic C-isotope fractionations in plants: A review

J Ghashghaie[1]**, and F-W Badeck**[2]

[1]Ecologie, Systématique et Evolution, Université Paris-Sud, CNRS, AgroParisTech, Université Paris-Saclay, 91400, Orsay, France

[2]Council for Agricultural Research and Economics, Genomics Research Centre, *via* San Protaso 302, Fiorenzuola d'Arda, 29017, Italy

E-mail: jaleh.ghashghaie@u-psud.fr

Abstract. C-isotope fractionation during post-photosynthetic processes mainly during respiration has received increasing interest during the last two decades. We have shown that leaf-respired CO_2 in the dark is in general ^{13}C enriched in all plant types (C3, C4, herbs and woody species), while root-respired CO_2 is ^{13}C depleted compared with organic material of respective organs (except in roots of woody species). Data from literature have also shown a huge variability in C-isotope fractionation during plant respiration of up to 15 per mil among species and with environmental conditions. We investigated the metabolic origin of the isotopic signature of respired CO_2 and its variability and demonstrated that for a given plant species, the heterogeneity in intra-molecular ^{13}C distribution in hexose molecules, relative activities of different metabolic pathways associated with respiration mainly those fixing (enzyme PEPc activity via anaplerotic pathway) or releasing CO_2 (pentose phosphate pathway, enzyme PDH reaction, and Krebs cycle), changes in respiratory pool sizes under different environmental conditions (drought, temperature, N-type nutrition, etc.) as well as the duration in the dark (beginning compared with end of the night, and mainly the light-to-dark transition time) are at the origin of the variability observed.

Plenary Pl-7

The necessity of guidelines of operations and maintenance for photovoltaic power plants

Chaengheon Kim, Cheolhyun Lim and Sukho Lee

[1] Green Energy R&D Department, Green Energy Institute, Mokpo, South Korea

E-mail: Chkim@gei.re.kr

Abstract. The importance of photovoltaic (PV) power plants installation is getting bigger not just because of the environmental issue but also the maintenance aspect. South Korean Ministry of Trade, Industry and Energy declared that it has been aimed over 20 % of national power generation rate of the country will be provided by renewable energies such as PV, wind power, etc., by 2030. The new installation of PV should be over 36.5 GW to meet the declaration thus the market of PV installation and maintenance will be energized. However, 14,314 malfunction reports have been reported from existing PV plants from year of 2013 to 2017, also there are over 50 fires annually from data collected during past 5 years. The installation of PV plant in the country is guided by the Korea Standard (KS) but there are no effective guidelines for the maintenance to guarantee not just for the safety but also the performance. In worldwide, IEC (International Electrotechnical Commission) has been launched IECRE PV-OMC (Operating Management Committee) for the renewable energies to establish guidelines for PV plants installation, maintenance and conformity assessment based on the IEC standards of PV system. In this study, it will be reported the necessity of the guidelines and standards for the maintenance and conformity assessments of PV plants. Also, recently ongoing projects of IECRE PV-OMC will be reported.

Plenary Pl-8

A study on linkage management of multi-microgrid based direct current supply of electric power

Chunsung Kim, Jongcheol Kim, Yukyeong Lee, Jaeha Ko

Green Energy Institute (GEI), 177 Samhyangcheon-ro, Mokpo-si, 58656, Republic of Korea

E-mail: minisung13@gei.re.kr

Abstract. Industrial complexes have different load characteristics and load time depending on the products of each factory, and thus various power can be utilized by using micro grid. In this study, we will construct a nano-grid with PV, ESS, PCS installed in each plant as a DC distribution, and discuss energy efficiency improvement through electricity trading in the micro-grid connected with nano-grid. The proposed system constructed the actual micro grid in the agricultural industrial complex and verified the algorithm through experiments. Through the linkage of each factory, energy is freely traded, and it aims to operate stably through various conditions of Peak-cut, Load shaving, and E-prosumer.

Plenary Pl-9

Proton Transfer Polymerization

A Khan

Department of Chemical and Biological Engineering, Korea University, 0231 Seoul, South Korea

E-mail: anzar@korea.ac.kr

Abstract. While an old reaction, the interest in thiol-epoxy reaction, especially as a polymerization process, is only recent. The power of this chemistry lies in its efficiency, operation under ambient conditions, commercial availability of a vast variety of thiol and epoxide carrying molecules that can be utilized as monomers, a long list of polymerization catalysts and associated solvent systems, and formation of a hydroxyl group upon completion. The amine-epoxy reaction bears similar hallmarks but is relatively simpler as a catalyst is not required for this process. The polymerization process itself is referred to as a 'proton transfer polymerization'. This is because quenching of the alkoxide anion, generated upon the nucleophilic attack of thiolate or amine moiety on the epoxide unit, through protonation is the critical step that ultimately decides the nature of propagation and the final structure of the polymer.Here, we will discuss the use of thiol/amine-epoxy chemistries as the polymerization process.

Plenary Pl-10

Neutron and X-ray methods for structure characterization

K D Knudsen

Institute for Energy Technology, 2027 Kjeller, Norway

E-mail: kenneth.knudsen@ife.no

Abstract. X-rays and neutrons are invaluable probes to explore material structure from the atomic to microscopic scales. So-called small-angle scattering (SAS) techniques are particularly useful for studying particle shape, size and interactions on the nanoscale. X-ray and neutron techniques complement each other in this respect due to varying sensitivity to different elements, as well as other factors. Some striking differences are the possibility for neutrons to penetrate thick metal containers and probe a material located inside, and the low characteristic energy of the neutron (typically meV) that precludes direct damage to chemical bonds. Several examples will be given of the applicability of these methods in material science, with a specific focus on the use of neutrons in the area of Soft Matter.

Plenary Pl-11

Energy Sources of Earth Mantle Dynamics

A Limare

Université de Paris, Institut de Physique du Globe de Paris, 1 rue Jussieu, 75005 Paris, France

E-mail: limare@ipgp.fr

Abstract. Convection in the Earth's mantle is largely driven by internal energy sources, involving heat released by the radioactive decay of long-lived isotopes Uranium, Thorium and Potassium and sensible heat extracted through secular cooling. The Earth's mantle is also heated from below by the Earth's core but the magnitude of the basal heat flux is not known precisely. I will show how laboratory experiments coupled to geophysical observations can contribute to a better understanding of the Earth's convective engine.

Plenary Pl-12

Quality control of purified proteins to improve research data reproducibility: improving the time-efficiency and quality of your results

A Matagne and The QC team of ARBRE-MOBIEU and P4EU

Laboratory of Enzymology and Protein Folding, Centre for Protein Engineering, University of Liège, Building B6C, Allée du 6 Août, 13, 4000 Liège, Belgium. amatagne@ulg.ac.be

Abstract. As the scientific community strives to make published research ever more transparent and reliable, the quality of biological reagents used comes into focus. One category of such reagents that requires much stricter quality controls are recombinant proteins. Examples of typical quality issues will be presented, along some results as to how this affects the reliability of the intended downstream application. In order to improve the reliability and reproducibility of data using purified proteins in life science research, a group of professionals involved in protein purification and protein characterization (in particular molecular biophysics) from both the ARBRE-MOBIEU and P4EU networks have drafted guidelines for improved quality control (QC). These guidelines, consisting of (i) minimal information to be provided about the protein identity, production parameters and long-term stability, (ii) a minimal set of quality tests for purity, homogeneity and identity, and (iii) some further recommendations (concerning e.g. DNA contamination, "spectral and thermal denaturation signatures", homogeneity, "competent fraction", storage conditions, batch-to-batch reproducibility, etc.) for tests based on the intended application of the proteins, will be presented. Furthermore, over a one-year period, the networks have attempted to evaluate the impact of these guidelines by correlating the levels of QC applied to given samples with the success and reproducibility of downstream experiments. The results indicate that QC guideline implementation can facilitate both experimental reliability and protein quality optimization. It seems, therefore, that investing in protein QC is advantageous to all the stakeholders in life sciences (researchers, editors and funding agencies alike) by improving data veracity and minimizing loss of valuable time and resources.

Plenary Pl-13

Aspects of structural investigations of 'Core-Shall' structures, $Fe_3O_4/CoFe_2O_4$, by X-Ray and Neutron Scattering

A Nagornyi[1,2], V Bodnarchuk[1], M Avdeev[1], O Ivankov[1], A Shulenina[3], A G Belous[4] and L A Bulavin[2]

[1] Joint Institute for Nuclear Research, Joliot-Curie str. 6, Dubna, Moscow reg., Russia, 141980
[2] Taras Shevchenko National University of Kyiv, Volodymyrska str. 60, Kyiv, Ukraine, 01033
[3] National Research Center «Kurchatov Institute», Ak. Kurchatova pl. 1, Moscow, Russia, 123182
[3] Vernadsky Institute of general and inorganic chemistry, pr. Ak. Palladina, 32/34, Ukraine, Kiev, 03142

E-mail: avnagorny@jinr.ru

Abstract. Synthesis of magnetic nanoparticles (MNPs), such as Fe_3O_4, $CoFe_2O_3$ etc., are of great interest because of the possibility of their wide using in technology and science, especially in medicine. For medical applications MNPs have to be nanosized, monodispersed, nontoxic and have stability to aggregation. The structural aspects of powders $Fe_3O_4/CoFe_2O_4$ magnetic nanoparticles with the anticipated "core–shell" structure have been analysed by comparison with individual Fe_3O_4 and $CoFe_2O_4$ particles using X-ray powder diffraction, small-angle neutron and X-ray (synchrotron) scattering. It is shown that MNPs in the powders are strongly polydisperse and form complex aggregates. The characteristic sizes of the crystallites, as well as the ratio between magnetite and cobalt ferrite in the composition of the $Fe_3O_4/CoFe_2O_4$ particles are estimated based on analysis of the diffraction peaks. Analysing the small-angle scattering data, the characteristics particles' size and aggregates are obtained. The fractal dimensions of the aggregates are determined. A significant difference between scattering at $Fe_3O_4/CoFe_2O_4$ particles and the total scattering derived from the partial contributions of scattering events at powders of separate magnetite and cobalt ferrite particles is observed, which suggests the formation of a "core–shell" structure.

Plenary Pl-14

Caracterization of pharmaceuticals, cosmetics and supplements using Stable Isotope Ratio Analysis

M Perini and S Pianezze

Fondazione Edmund Mach, via Mach1, 38010, S. Michele all'Adige, Italy

E-mail: matteo.perini@fmach.it

Abstract. Stable isotope ratio analysis of bio-elements (hydrogen, carbon, nitrogen, oxygen and sulphur) has been used since the 1990s to check food authenticity and traceability of a wide variety of food commodities. In the last years, examples of applications also in the pharmaceutical and cosmetic field have been reported. The use of stable isotope analysis for products authentication purposes is possible thanks to isotopic fractionation occurring in several processes and reactions (biological, biochemical, physical, chemical etc.) which generates unique isotopic signatures. For this reason, the application of this technique on the bulk samples as well as on specific components (e.g. aroma compounds) can be used to detect the origin of an ingredient (synthetic or natural), the substitution of one ingredient for another, as well as the geographical and/or botanical origin of the products. The $\delta^{13}C$ and $\delta^{2}H$ values of vanillin can determine whether the product is natural (deriving from the expensive CAM plant *Vanilla*), biotechnologically derived or synthetic. Moreover, the $\delta^{13}C$ values of specific components of *Rosa damascene mill*., one of the most expensive essential oils in the market world, can indicate the fraudulent addition of cheaper oil from a C4 plant (e.g. *Cymbopogon martinii, palmarosa*). In pharmaceutical and cosmetic formulations, $\delta^{13}C$ analysis is a suitable tool to discriminate between squalene and squalane from shark (illegal) and from olive oil (expensive) as well as between monacolin K (contained in the fermented dietary supplement red yeast rice) and the commercially marketed statin, lovastatin. It's possible to combine different isotopic signatures to guarantee the natural origin of curcumin, caffeine, tartaric acid and its derivatives. These examples demonstrate that the isotopic fingerprint represent an effective tool for the authenticity assessment of economically important pharmaceutical, cosmetic and supplement products.

Section T1:

Stable Isotopes, Labeled Compounds and Analytical Techniques

Oral T1-1

Raman analysis - perspective for innovative polyamide composites

I Brezestean[1, 2], D Marconi[1], A Colniță[1], R Pasca[1, 2], A A Mâinea[3], N Levința[3]and I Turcu[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]Babes-Bolyai University, Faculty of Physics, Biomolecular Physics Department, Cluj-Napoca, Romania

[3] National Institute for Research and Development in Chemistry and Petrochemistry, Department of Polymers, 060021, 202 Spl. Independentei, Bucharest, Romania

E-mail: Ioana.Brezestean@itim-cj.ro

Abstract. Polyamides represent a class of thermoplastic polymers with multiple industrial applications for advanced manufacturing industries. Satisfying industrial needs in terms of mechanical characteristics has led to the development of composite materials. Our main target was to introduce different fillers, such as graphene or layered double hydroxides, into the polyamide matrix, in order to improve the existing mechanical properties. In this work we present a Raman characterization of a new bio-based polyamide (with low CO_2 footprint) loadedwith graphene nanoplatelets. The potential of the Raman spectroscopy was used also to investigate composite structures obtained with layered double hydroxides. A complete Raman analysis of specific groups was investigated over neat polyamide and polyamide composites exposed at different thermal treatment in order to analyze the influence of environmental conditionsAnalysis of G, D and 2D Raman peaks and the relative intensity ratio I_D/I_G, revealed the fact that a higher concentration of graphene in polyamide is suitable for improving the essential physical properties and also decrease the defects in the graphene layers. **Acknowledgements**. This work was supported by a grant of the Romanian Ministery of Research and Innovation, CCCDI – UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0387 / 80PCCDI/2018, within PNCDI III.

Oral T1-2

Classification of Transylvanian cheese using isotopic and elemental profiling

D A Magdas, I Feher, G Cristea and C Voica

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: alina.magdas@itim-cj.ro

Abstract. This study presents the classification of Transylvanian cheese, according to the geographical origin and also, with respect to species (cow vs. sheep), of two traditional specialties, salty and ripened cheese. To achieve this goal, the elemental profile along with carbon isotopic ratios ($^{13}C/^{12}C$) of cheese and extracted casein were corroborated through chemometric methodsin order to obtain the best differentiation markers. Data processing was performedusing SPSS Statistics 24 (IBM, USA). Fifty-seven descriptors were measured in 66 cheese samples purchases from three different Transylvanian producers. The statistical procedures used in this study were Pearson correlation and linear discriminant analysis (LDA). By applying the proposed approach, a differentiation better than 92% for geographical origin of investigated cheese was obtained having as the most powerful predictors the isotopic composition of casein ($\delta^{13}C_{casein}$) along with Sr, Li, Mg, Rb and K. Forthe species differentiation (cow vs. sheep) a separation of 100% in both initial and cross-validation procedure was achieved. In this case the most important markers proved to be Li, Cs, Mg, Ga, Nb, Sr and Ca concentrations. **Acknowledgment**: The financial support for this work was provided by the Ministry of Research and Innovation, Core Program, contract no. PN 19 35 02 02

Oral T1-3

Assessment of reaction intermediates in biomolecular systems using isotope exchange effect

A C Mot[1,2] and C Zagrean-Tuza[1,2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donath, 400293 Cluj-Napoca, Romania

[2]Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemistry, 11 Arany Janos, 400028 Cluj-Napoca, Romania

E-mail: augustin.mot@itim-cj.ro

Abstract. A reaction intermediate is a transient and usually short-living chemical speciesformed during a reaction that involves several steps. Most of the reactions observed in biological systems imply multi-step reactions which contain intermediates that might convey important information regarding the reaction mechanisms. Once the reaction mechanism is known, one may efficiently intervene and control its fate, either by preventing some undesired results such as disease control using inhibitory drugs or accelerate it by a suitable effector. In this study, we discuss the efficiency of the protium-deuterium exchange in aqueous solution in order to identify the structure of the radicals that are generated from natural polyphenols, enzymatically or chemically by alkali treatment using electron paramagnetic resonance spectroscopy. Moreover, reaction mechanism of nitrite and hydroxylamine reduction by non-symbiotic plant hemoglobins were investigated exploiting ^{15}N isotope effect.

Oral T1-4

Raman spectroscopy analysis of metal-ferrite nanoparticles: towards precise interpretation and extraction of structural information

F Nekvapil[1,2], A Bunge[1], T Radu[1], S Cintă Pinzaru[2] and R Turcu[1]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies Cluj-Napoca, Physics of Nanostructured Systems Department,67-103 Donat, 400293 Cluj-Napoca, Romania

[2]Babeş-Bolyai University, Biomolecular Physics Department, Kogălniceanu 1, 400084 Cluj-Napoca, Romania

E-mail: fran.nekvapil@itim-cj.ro

Abstract. A robust interpretation framework for extraction of structural information based on Raman spectra of spinel structured $Mn_{(1-x)}Zn_xFe_2O_4$ nanoparticles (NPs) is discussed. Since ferrite NPs give rise to complex Raman modes, their interpretation requires careful consideration on the Raman scattering in solids at nanoscale. Presently, there is no common approach, resulting in inconsistent and incomplete interpretation of Raman spectra of ferrite NPs across studies. The proposed framework is being developed by recording and comparing Raman spectra of our own Mn-Zn-ferrite NPs obtained under various synthesis conditions, of iron oxide NPs, and data found in literature. The spectral feature stretching from about 600 to 800 cm^{-1}, termed A_{1g} band, gives information on tetrahedral crystalline sites. Correct deconvolution by applying the appropriate functions and number of peaks for each Raman band results in highly consistent peak positions, thus improving our capability to relate parameters of Raman bands to structural properties of ferrite NPs. **Acknowledgement.** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0062, contract no. 58, within PNCDI III.

Oral T1-5

The identification of materials used by Dumitru Ispasto paint the Straja wooden church, Cluj County

D Nemes[1], C Marutoiu[1], I Bratu[2], C Neamtu[3], I Kacso[2], O F Nemes[1] and I Udrea[4]

[1] *"Babes-Bolyai"* University, Faculty of Orthodox Theology, N. Ivan St., 400692 Cluj-Napoca, Romania

[2]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[3]Technical University of Cluj-Napoca, 28 Memorandumului, 400116, Cluj-Napoca, Romania

[4] *"Babes-Bolyai"* University, Faculty of Chemistry and Chemical Engineering, 11Arany Janos, 400028 Cluj-Napoca, Romania

E-mail: D_nemes2000@yahoo.com

Abstract. Straja is a village documented since 1219 (Gnezted). It hosts an interesting historical monument, the Church of the Archangels Michael and Gabriel, built at the beginning of 18th century. The church is built from fir wood placed on an oak base. The construction consists of the altar, nave and narthex. The mural painting of the church was executed by the painter Dumitru Ispas from Gilau, in collaboration with his son Ştefan. The materials used by the two artists were investigated by XRF spectroscopy, FTIR spectroscopy and DSC calorimetry. The painting was applied on a thin layer of primer and hemp canvas strips were applied at the beams joining places. The identified materials are: gypsum, animal glue, egg yolk, red lead, red iron, malachite green and orpiment. **Acknowledgments:** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI—UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0812/53PCCDI, within PNCDI III

Poster T1-1

Production and application of stable isotopes

D Axente

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat Str., 400293 Cluj-Napoca, Romania

E-mail: Damian.Axente@itim-cj.ro

Abstract. The main applications of stable isotopes: D, ^{7}Li, ^{10}B, ^{13}C, ^{15}N, ^{17}O, ^{18}O in medicine, biology and pharmacology are presented. For positron emission tomography (PET) the isotopes: ^{18}O, ^{13}C, ^{15}N are commonly used for discovery of the malignant tumours in order to establish the treatment. The production of stable isotopes ^{13}C, ^{18}O, ^{15}N has grown steadily by about 2% per year between 1940 and 2000, reaching a volume of about 1200 Kg/year ^{18}O and about 600 Kg/year ^{13}C in the year 2015. For these isotopes is provided a production increase so that in 2020 will be reached a volume of about 2000 Kg/year of ^{18}O and about 700 Kg/year of ^{13}C. It is expected that in 2022 the global stable isotope and labelled compounds market will reach 294.2 million USD from 254.6 million USD in 2017, at an annual growth rate of 2.94%. The world's leading manufacturers of ^{13}C are presented, the most applied method being the cryogenic rectification of carbon monoxide. In the case of ^{18}O the most applied production method is the rectification of water under vacuum. The world's main producer of ^{15}N is China and the isotopic exchange method in nitrogen oxides – nitric acid system (Nitrox) is practically unanimously applied after ^{15}N production plants using cryogenic rectification of nitric oxide in USA and probably in Georgia were shut off, due to the repeated explosions. The method of ^{15}N/^{14}N exchange in Nitrox system remains the only alternative for industrial scale production of ^{15}N in view to use this isotope for production of nitride type nuclear fuels (U^{15}N, Pu^{15}N) for advanced nuclear reactors.

Poster T1-2

Multivariate statistical approach for advanced verification of vegetables growing regime based on mineral profile

O R Botoran, R Popescu, A M Radulescu, C Sandru, M Iordache, D Costinel and R E Ionete

National Research and Development Institute for Cryogenics and Isotopic Technologies- ICSI Rm. Valcea, 4 Uzinei, 240050 Ramnicu Valcea, Romania

E-mail: oana.dinca@icsi.ro

Abstract. Discrimination among two agricultural farming systems (conventional and organic) was performedin this study by combining mineral profiles (K, Ca, Na, Mg, Fe, Zn, Cr, Ni, Pb, As, Cu, Cd, Co, Al, Mn, Rb and Sr) of 89 vegetables samples with several statistical modelling approaches. Comparative statistical tests of the elements concentration mean values show significantly ($p < 0.05$) different levels of Cr, Ni, Pb, Cu, Co, Mn, Rb, Sr, Zn and Ca between the organically and conventionally grown vegetables; achievement of approximately 59% significant variability among all elements at a 95% confidence level, denotes a clear difference between the two growing regimes.Pattern recognition techniques were used to reveal similaritieswithin groups and develop classificationmodels.By modelling the data using principal component analysis we obtained 51% of the total variance explained and a 92%successful classification rate for the discriminant analysis, highlighting the potential of the elemental profile to discriminate among the two groups according to the cultivation method. Within the framework of this study, systematic differences in the concentrations of certain elements had occurred between organically and conventionally grown vegetables, suggesting that elemental profile may be useful as indicator of the cultivation regime.

Poster T1-3

Analysis of painting materials from "The Lord's Transfiguration" icon painted by Grigore Ranite

I Bratu[1], C Marutoiu[2], D Nemes[2], D Toader[3], O F Nemes[2] and R Suciu[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]Babes-Bolyai' University, Faculty of Orthodox Theology, N. Ivan St., 400692 Cluj-Napoca, Romania

[3]Ethnographic Museum of Transylvania, 21 MemorandumuluiSt., 400114 Cluj-Napoca, Romania

E-mail: ibratu@itim-cj.ro

Abstract. The materials used by the painter Grigore Ranite to create the "**The Lord's Transfiguration**" icon were analyzed by: XRF spectroscopy and destructive and non-destructive FTIR spectroscopy. The primer of the icon was made using gypsum and animal glue. The red color used is red lead mixed with red mercury. For brownish red the painter used realgar and litharge (lead red). Green malachite was also used. Brown and ochre contain iron oxide. Gold leaf was also used. .Binder: egg yolk. The panel on which the icon was painted is made of fir tree which had hemp canvas applied over it. **Acknowledgments** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI—UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0812/53PCCDI, within PNCDI III

Poster T1-4

New insights into polydopamine structure using a combined $^{13}C/^{1}H/^{2}H$ solid-state NMR study on deuterated samples

M V Cîrcu and C Filip

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: monica.circu@itim-cj.ro

Abstract. Despite the large number of applications reported for polydopamine (PDA), there is still a fundamental challenge remained in the field: no complete structure elucidation of PDA is available to date. Acknowledging the fact that this comes from the limitations of standard analytical techniques when applied to such complex and heterogeneous systems, a solid-state NMR approach was introduced, which brings important novelties with respect to both, sample engineering and the employed experimental techniques. ^{2}H solid-echo, ^{1}H fast-MAS and ^{1}H Double-Quantum filtered ss-NMR experiments on PDA samples prepared under three different deuteration schemes are reported for the first time in the present work. Their results, together with the results of ^{13}C CP-MAS/CPPI ss-NMR experiments at 25 kHz MAS, provide key structural and dynamical information, capable to removesome of the uncertain structural characteristicsstill present the literature data on PDA.

Poster T1-5

Sources and ecological risk assessment of PAHs in the sediments of Olt River, Romania

C Ciucure and E-I Geana

National Research and Development Institute for Cryogenics and Isotopic Technologies – ICSI Ramnicu Valcea, 4 Uzinei, 240050 Ramnicu Valcea, Romania

E-mail: irina.geana@icsi.ro

Abstract. The aim of the study was to assess the concentration, sources and ecological risk of PAHs (polycyclic aromatic hydrocarbons) in sediments collected from elevenartificial lakes on the middle and lower course of the Olt River, Romania. The total concentrations of PAHs (ΣPAH) in sediments varied from 0.0239-4.5998 mg/kg dry weight. Distribution patterns and source identification results indicated that the PAHs under study in these areas were mainly derived from pyrolytic and petrogenic sources. PCA analysis based on PAHs profile and some ratios between them (Phe/Ant, Fla/Pyr, BaA/(BaA+Chr), Flua/(Fla+Pyr)) allow the discrimination of the sampling sites depending on the degree of contamination. Although the concentration of acenaphthene, anthracene and fluoren in sediments exceeded the ERL level in some sampling areas, the mean ratio of the ERL showed a relatively low level of toxicity in these sediments, except for two locations.At the same time, the effects of the average ERM coefficient showed that the 15 polycyclic aromatic hydrocarbons analyzed in the sediments of Olt river, Roumania, present an ecological reduction of the risk. Toxicity and biological risk were assessed using the equivalent amount of toxicity (TEQ) and the sediment quality coefficient (SQG). Contamination of sediment-based PAHs can turn into environmental hazards in two locations categorized as moderately polluted sites.

Poster T1-6

The CHN stable isotope signatures coupled with physicochemical parameters in authentication the raw material from commercial honey

D Costinel, R E Ionete, O R Botoran, I E Geana and C T Ciucure

National Research and Development Institute for Cryogenics and Isotopic Technologies – ICSI Rm. Valcea, 4 Uzinei, 240050 Ramnicu Valcea, Romania

E-mail: diana.costinel@icsi.ro

Abstract. The authenticity of honey pursues two objectives: the naturalness (pure honey, not adulterated with inverted molasses or syrups from sugar cane or beet) and authenticity, in terms of botanical and geographical origin. The aim of this study was to assess the raw material from commercial honey using the signature of CHN stable isotopes ($\delta^{13}C$ and D/H in ethanol from fermented honeys, $\delta^{13}C$ and $\delta^{15}N$ from honey protein and $\delta^{13}C$ from honey) coupled with physicochemical parameters (e.g. Brix, pH, refractive index RI, acidity, electrical conductivity). Also, adulterated honey samples, with different sugar syrup additions from 10% to 30% were investigated to validate our findings. Principal component analysis (PCA) was applied to study which variables are the most important for honey samples separation according to their geographical and botanical origin. The results showed that CHN stable isotope fingerprint could be used as indicator for honey naturalness, varietal classification and provenance of origin.

Poster T1-7

Method for the extraction and quantification of fatty acid distribution in edible vegetable oils

F D Covaciu, D A Magdas and Z Moldovan

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: florina.covaciu@itim-cj.ro

Abstract. Edible vegetable oils vary widely in the chemical composition. Fats are composed of a mixture of either saturated, monounsaturated or polyunsaturated fatty acids in different concentrations. The quality of oils is determined by the spectrum of fatty acids and is grouped according to the prevailing fats. Edible vegetable oils are largely made up of fats (lipids and triglycerides of fatty acids), small amounts of vitamins (vitamin E, A and D) and adherents as phosphatides (lecithin and cephalides), unsaponifiable substances and other free fatty acids obtained from vegetable oilseeds. Determination of fatty acids in oil samples presents some basic difficulties, such as: efficient extraction of fatty acids from the oil sample, chromatographic separation of the corresponding fatty acid andthe detection with high sensitivity for quantitative analysis. The amount of fatty acids in oil samples varies, therefore requires the development of efficient extraction methods in a wide range ofconcentrations.The aim of the paper is detection and measurement of fatty acids from complex mixtures. The determination of 37 fatty acids with diferent unsaturated degree is obtined using the GC having FID detector. The compounds were analyzed as methyl esters of the corresponding fatty acids. **Acknowledgment**: The financial support for this work was provided by the Ministry of Research and Innovation, program Nucleu, contract no. PN 19 35 02 02.

Poster T1-8

Isotopic and elemental profiling alongside with chemometric methods for pork chop samples differentiation

G Cristea, C Voica, R Puscas, D A Magdas, I Feher and S Radu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: gabriela.cristea@itim-cj.ro

Abstract. In the context of product markets globalization and rapid transportation of food across countries, the possibility of mislabeled products increases. Thus, consumers prefer to pay a higher price for food products, including meat, from a specific region. The meat products represent an important component of human diet, being one of the most valuable sources of nutrients, and offering different essential elements. Mass spectrometry is a powerful technique in the field of food authentication. In this study, 93 pork chop samples were analyzed from isotopic ($\delta^{13}C$, $\delta^{18}O$, and $\delta^{2}H$) and elemental point of view, in order to investigate the regional origin of these products and trace pork diet. Statistical methods were used to: i) highlight significant regional differences among studied parameters and to identify the best discrimination markers for pork meat origin; ii) determine the best predictors for animals feeding. The isotopic composition of oxygen and hydrogen was determined from the water extracted from meat samples, by cryogenic distillation without isotopic fractionation. $\delta^{18}O$ and $\delta^{2}H$ values ranged from -8.6 to -2.1 ‰, and from -67.4 to -20.2 ‰, respectively. The isotopic fingerprint of carbon varied between -25.6 to -14.7 ‰. **Acknowledgment**: The financial support for this work was provided by the Ministry of Research and Innovation, program Nucleu, contract no. PN 19 35 02 02.

Poster T1-9

Variability of elemental and isotopic content of different animal tissues

A Dehelean, D A Magdas, G Cristea, I Feher, F Covaciu and R Puscas

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: abenta@itim-cj.ro

Abstract. The determination of multielement concentrations in foodstuffs is important in different fields including nutrition and toxicology. Some metals (Fe, Mn, Cu, Se, etc.) are known to be essentials and other with potentially toxic (Al, As, Cd and Pb) which can influence the quality of the products. The contents of these elements seem to vary among the species or animal tissues. Also, the different feeding modes can influence the nutritional or toxic value of meat. The principle of differentiation of samples having different origin, by using $\delta^{18}O$ and $\delta^{2}H$, is based on the variation of these isotopes in the precipitation, with distance from the sea and temperature being the main factors. Also, the use of stable carbon isotopes to identify corn-fed pork and chicken is based on the fact that the $^{13}C/^{12}C$ stable isotope ratio of corn being a C4 plant is significantly different from the $^{13}C/^{12}C$ stable isotope ratio of wheat, which is a C3 plant. This study was aimed to determine the elemental profiling and isotopic content in different cuts of pork, beef and chicken collected from supermarkets and butcheries in Romania. The experimental data were subjected to statistical techniques using ANOVA, PCA and DA classification. **Acknowledgment**: The financial support for this work was provided by the Ministry of Research and Innovation, program Nucleu, contract no. PN 19 35 02 02.

Poster T1-10

Preoperational Monitoring of Experimental Pilot for Tritium and Deuterium Separation-ICSI. Radioactivity concentration in surface water

M R Ene, I S Spiridon, G Bulubasa and A Miu

National Research and Development Institute for Cryogenics and Isotopes Technologies, 4 Uzinei, 240050, Ramnicu Valcea

E-mail:mihaela.ene@icsi.ro

Abstract. The paper presents a monitoring activity of the surface water radioactivity variation around the Experimental Pilot Plant for Tritium and Deuterium Separation (PESTD) over an experimental campaign of 1 year. The main purpose of the radioactivity monitoring of the environmental factors in the preoperative stage is to establish the levels of radioactive concentrations in the environment. Two surface water sampling points for the Olt River were chosen, the first one in upstream of the discharge point of the magistrate channel "Deversor Olt" and respectively the second sampling point in downstream of the liquid effluents discharge point. The level of natural background radiation was established by collecting water samples at a minimum distance of 15 km from the PESTD unit perimeter, distance considered not influenced by the radioactivity of the facility.Activity concentration of radionuclides measurements were performed in surface water from sampling points establish on the Olt River near the magistrate channel "Deversor Olt" on a weekly frequency basis. The method used was high resolution gamma ray spectrometry performed with a HPGe detector.

Poster T1-11

Edible oils evaluation using fat soluble vitamins (FSV) content

I Feher, O Marincas, V Floare-Avram, F Covaciu and D A Magdas

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: ioana.feher@itim-cj.ro

Abstract. The quality and authenticity of edible vegetable oils is an important issue, for both consumers and producers, due to their impact on health, but also from economical and commercial considerations. From nutritional point of view, edible oils represent a source of energy, providing essential fatty acids, considered an excellent carrier medium for oils soluble vitamins (A, D, E and K). In this work, a high-performance liquid chromatography (HPLC) with UV detector was developed, for the identification and quantification of FSV from edible oils. By applying the developed method, it was revealed that the higher concentration was found for vitamin E. The obtained results were used further for development of chemometric model, by applying linear discriminant analysis (LDA), able to differentiate the oils according to their species (sun flower, olive, pumpkin, grapeseed oils) and their production process (cold pressed versus refined). **Acknowledgment**: The financial support for this work was provided by the Ministry of Research and Innovation, program Nucleu, contract no. PN 19 35 02 02.

Poster T1-12

Comprehensive evaluation of tomatoes using pesticides, phenolics, multielemental and isotopic content

V Floare-Avram, F Covaciu, C Voica, R Puscas, I Feher, O Marincas and A Magdas

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: veronica.avram@itim-cj.ro

Abstract. Tomato (*Solanum lycopersicum L.)* is the second most important vegetable crop in the world, next to potato, with a worldwide harvest of over 162 million tons annually. It is an excellent source of many nutrients and secondary metabolites that are important for human health, including mineral matter, vitamins, lycopene, flavonoids, organic acids, phenolics and chlorophyll. The presence of nutritiveand toxic elements in tomato samples depends on the growing conditions and the utilization of pesticides and fertilizers. In the last century, new agricultural technologies and the massive use of chemical fertilizers, pesticides and herbicides provided an increased productivity at lower prices. The present study aims to compare the influence of geographic origin and agricultural practices on tomato fruit composition. For this purpose, 41 samples of tomato fruit were investigated from the point of view of: phenolic compounds, isotopic values (^{18}O, ^{13}C, ^{2}H), elemental profile and pesticides. Using investigated parameters, stepwise linear discriminant analysis (SLDA) was applied in order to highlight the differences that occurred between organic and conventional grown tomatoes, and also between Romanian and abroad purchased samples. **Acknowledgment**: The financial support for this work was provided by the Ministry of Research and Innovation, program Nucleu, contract no. PN 19 35 02 02.

Poster T1-13

Electrochemical biosensing of phenolic compounds from wines

E I Geană[1], V Artem[2] and C Apetrei[3]

[1] National Research and Development Institute for Cryogenics and Isotopic Technologies – ICSI Rm. Valcea, 4 Uzinei, 240050, Ramnicu Valcea, Romania

[2] Research Station for Viticulture and Oenology Murfatlar, Calea Bucuresti str., No. 2, Murfatlar, Constanta, Romania

[3] "Dunarea de Jos" University of Galati, Faculty of Science and Environment, Department of Chemistry, Physics and Environment, 47 Domneasca Street, Galati, Romania

E-mail: Constantin.Apetrei@ugal.ro

Abstract. A multicomponent enzyme sensor based on screen-printed carbon electrode modified with cobalt(II)phthalocyanine (CoPc) as electron mediator and tyrosinase as biocatalyst was used for the evaluation of phenolic compounds and antioxidant activity of white and red wines. Tyrosinase was immobilized on the screen-printed Co-phthalocyanine carbon electrode (CoPc-SPC) by casting technique followed by cross-linking. Amperometric measurements were recorded at an applied potential of 0.050V versus Ag pseudoreference electrode, while cyclic voltammograms were registered from −1.0 to +1.0 V, at 0.1 V/s sweep rate (with integrated counter electrode - carbon and reference electrode-silver). Amperometric biosensor allows the quantification of polyphenols from wine at a low applied potential value, reducing the effect of interfering compounds. Analytical characteristics of proposed Ty/CoPc-SPC biosensor were evaluated towards gallic acid and the effect of sample matrix composition on the response of the sensor was studied. The modified Ty/CoPc-SPC sensor was used for the analysis of wines after a pre-treatment step in order to minimize the influence of sulphur dioxide. The biosensor gave good results when employed for wine analysis, showing a good agreement with the spectrophotometric measurements by Folin-Ciocalteu method, the official method for polyphenols' analysis in wine. A good correlation was obtained between the wine phenolic content and the antioxidant activity of wines estimated by the DPPH spectrophotometric method.

Poster T1-14

Simultaneous GC-MS analysis of pharmaceutical active compounds from environmental and biota samples: uptake potential determination for common vegetables

D E Kovacs[1,2], L Silaghi-Dumitrescu[2], M H Kovacs[1] and C Roman[1]

[1]Research Institute for Analytical Instrumentation, 67 Donath, 400293 Cluj-Napoca, Romania

[2]Chemistry and Chemical Engineering Faculty, 11 Arany Janos, 400028, Cluj-Napoca, Romania

E-mail: dalma.kovacs@icia.ro

Abstract. Although at low concentration, pharmaceutical active compounds continuous introduction into the environment from different pathways makes them 'pseudo-persistent'. At moment it is unknow their potential transfer into crops and vegetables. This is mainly due to complexity of analytes and samples matrices. Because nonsteroidal anti-inflammatory drugs are frequently reported in environment, the aim of this study was to improve current analytical methods of analysis, and to assess their uptake potential in common vegetables as tomato, radish and salat. Samples ultrasound assisted extraction in large SPE column, followed by derivatization allowed their analysis at GC-MS with limits of detection between 0.02 – 0.5 $ng \cdot kg^{-1}$ for ibuprofen, ketoprofen and diclofenac. Factors as root concentration (RCF), translocation (TF) and bioconcentration (BCF) were determined to could establish these pharmaceuticals uptake potential by studied vegetables. Usually diclofenac BCF was the highest in case of all vegetables, between 31 – 118. Ibuprofen was easily accumulated in radish and salat, with levels between 6 – 58 and 11 – 73 $ng \cdot kg^{-1}$.

Poster T1-15

Biomonitoring of atmospheric metal pollution using *Thuja occidentalis* leaves

L Levei[1,2], O Cadar[1], E Kovacs[1,3], I Torok[1] and A Ozunu[2,4]

[1]INCDO-INOE 2000, Research Institute for Analytical Instrumentation, 67 Donath, 400293 Cluj-Napoca, Romania

[2]Babes-Bolyai University, Environmental Science and Engineering Faculty, 30 Fantanele, 400294 Cluj-Napoca, Romania

[3]University of Agricultural Sciences and Veterinary Medicine, 3-5 Manastur Street, 400372, Cluj-Napoca, Romania

[4]University of the Free State, DIMTEC, 205 Nelson Mandela Drive, 9300 Bloemfontein, South Africa

E-mail: levente.levei@icia.ro

Abstract. Air pollution with metals posesan important risk for human health, as it is associated with high incidence of respiratory, cardiovascular and neoplastic pathologies. Along the direct determination of metals concentration in air, the biomonitoring approach using plant or tree species allows the identification of polluted and unpolluted areas, especially in cities, where the atmospheric metal contents can vary widely in short distances. Northern white-cedar (*Thuja occidentalis*) is an evergreen tree widespread in cities that requires low maintenance and has ornamental and curtaining roles. In this study Thujawas used as a biomonitor of air pollution with Cu, Pb, Zn, Cr and Ni, by analysing these metals in the leaves of Thuja from areas with high and low traffic in Cluj-Napoca. The obtained results revealed no significant differences in the average content of Pb and Cr in the two studied areas and two times higher content of Cu, Zn and Ni in the high samples collected near roads with intense traffic. These results indicate that traffic could be a source of Cu, Zn and Ni in urban areas.

Poster T1-16

Optimization of the berries extracts with antioxidant activity

I Lung[1], M L Soran[1], O Opris[1], A Stegarescu[1], S Gutoiu[1], M Stan[1] and R Podea[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat Street, 400293 Cluj-Napoca, Romania

[2] S.C. Etera Prod S.R.L., 407281 Luna de Sus, Cluj, Romania

E-mail: ildiko.lung@itim-cj.ro

Abstract. The aim of this work was to obtain the extracts of the sea buckthorn and blackthorn by refluxing and ultrasound extraction. In order to obtain a high antioxidant activity of these extracts, central composite design (CCD) was employed to optimize the extraction parameters. The parameters taken into account were: the extraction time (30 – 150 min) and the water: ethanol ratio (60:40 – 20:80, v/v) for refluxing and the extraction time (5 – 30 min), temperature (30 – 70°C) and the water: ethanol ratio (60:40 – 20:80, v/v) in the case of ultrasound extractionwere optimized. The DPPH (2,2-diphenyl-1-picrylhydrazyl) method was applied for the antioxidant activity evaluation. It was observed that the highest antioxidant capacity of the sea buckthorn extract (300.81 mM Trolox/g dry vegetable material)was obtained by refluxing with water: ethanol (50:50, v/v) over a period of 102.43 min, while the highest antioxidant capacity (63.18 mM Trolox / g dry vegetable material) of the blackthorn extract was obtained by ultrasound extraction with water: ethanol (60:40, v/v) for 10 min at 66.82°C.

Poster T1-17

Kinetics of Chromium (IV) adsorption from aqueous solution, using Dowex-Marathon anionic resin

C Marcu, C Varodi and A Balla

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: cristina.marcu@itim-cj.ro

Abstract. In the present study, batch experiments were performed to remove chromium (VI) from aqueous solution, using Dowex-Marathon resin. In order to investigate the kinetic mechanism which controls Cr(VI) adsorption, four kinetic models were used: pseudo-first order, pseudo-second order, Elovich equation and intraparticle diffusion model.On reaction with 1,5 diphenyl carbazide, Cr(VI) forms a 1,5 diphenyl carbazide - Cr(VI) complex, which is analyzed at 540 nm, using UV-1800 Shimadzu spectrophotometer, after 7 minute. The Cr(VI) adsorption process was well described by the pseudo-second order kinetic model, for 0.1-0.3 g/L Cr(VI).

Poster T1-18

Quality assessment of lavender essential oils collected from various Romanian local producers

O Marincaş, I Feher, V Floare-Avram and D A Magdas

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: olivian.marincas@itim-cj.ro

Abstract. The quality of the oil produced from lavender (*Lavandula angustifolia L.)* is extremely important from several points of view, i.e. the classification and labelling of essential oils, identification of adulterated products, diluted oils labelled as being a higher-quality. The chemical composition of the samples was determined using gas chromatography coupled with mass spectrometry (GC/MS) and the quality evaluation was achieved by applying the new algorithm developed in a previous work. This approach allowed the classification of lavender oils as high, medium or low quality, without using the time consuming and expensive techniques such as quantitative analysis. A quality scale was also build based on correlation between the percentage abundance of each specific compound with concentration of the oil, to establish a grade for each product (from one to ten). **Acknowledgment**: The financial support for this work was provided by the Ministry of Research and Innovation, program Nucleu, contract no. PN 19 35 02 02.

Poster T1-19

Detection of Meldonium used in conjunction with other betablocker drugs forbidden for athletes

D Rusu[1], I Bratu[2], C Marutoiu[3], Z Moldovan[2] and M Rada[4]

[1]Iuliu Hatieganu University of Medicine and Pharmacy, Faculty of Medicine, 4 Louis Pasteur, 400349 Cluj-Napoca, Romania

[2] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[3]Babes-Bolyai University, Faculty of Orthodox Theology, f/n N Ivan, 400119 Cluj-Napoca, Romania

[4]Victor Babes University of Medicine and Pharmacy, Faculty of Medicine, 2 Eftimie Murgu, 300041 Timisoara, Romania

E-mail: cmarutoiu@yahoo.com

Abstract. A rapid method based on Fourier Transform Infrared Spectroscopy (FTIR) for the detection in urine samples of the forbidden conjunction use of Meldonium with some other beta blockers (Metoprolol, Amlodipine, Bisoprolol, Nebivolol, Betaxolol, Carvediol) for athletes was proposed. A TLC plate coated with SiO_2 was employed. A simple analytical method for screening the Meldonium and the mentioned beta blockers in urine samples by employing the TLC chromatographic plates, FTIR spectroscopy (with the aid of KBr pellet technique) and mass spectrometry was reported. The use of surface hydroxyl groups for the indirect detection of Meldonium in urine samples was proposed. Also, Meldonium was identified on the TLC plates by mass spectrometry.

Poster T1-20

Analysis of phthalates from medical devices and their release in artificial body fluid by GC-MS

S Mirel[1], Z Moldovan[2] and V Mirel[2]

[1]Iuliu Hatieganu University of Medicine and Pharmacy, Department of Medical Devices, 8 Victor Babeş, 400012 Cluj-Napoca, Romania

[2]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donath, 400293 Cluj-Napoca, Romania

E-mail: valentin.mirel@itim-cj.ro

Abstract. In the last years, the information concerning the safety of certain medical devices containing phthalates (used as plasticisers, which known or presumed carcinogenic, mutagenic or reprotoxic potential in humans) has been an important topic. Therefore, it is required to verify thesecompounds release from a device during medical procedures. The aim of this paper is to identify and quantify the present phthalates in some medical devices (as risk factors for patients and health professionals) and to study their potential migration towards body fluids. For phthalates determination a sensitive and selective method based on a gas chromatograph-mass spectrometer coupled system (GC/MS) was used. The detection limit is to level of low ng/ml of compound. The compounds were determined in different samples collected and a significant difference was observed among the migratory levels. The results are an important base in the study of migration process of the chemicals from medical device to living body.

Poster T1-21

Determination of light hydrocarbons in water samples from Black Sea by GC methods

Z Moldovan[1], F Covaciu[1], G Ion[2] and I Turcu[1]

[1]National Institute for R&D of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]National Institute for R&D of Marine Geology and Geoecology, 23-35 D. Onciul, 024053 Bucharest, Romania;

E-mail: zaharie.moldovan@itim-cj.ro

Abstract. In the last decade the interest in the environmental distribution of the methane has been increasing with purpose in investigation of unconventional gas sources or for studying the global warming processes. Analysis of the volatile hydrocarbons dissolved in water is very important in evaluating anaerobic activity and investigating the sources of contamination in aquatic environments. A sensitive and selective gas chromatographic method has been developed for analysis of dissolved methane, ethane, propane butane, pentane and hexane in marine water. For this purpose, a headspace method was developed. The dissolved methane, concentrations in the liquid phase were calculated using Henry's Law and partial pressures in the gas phase. The method needs minimal operation in sample preparation and offers low ng/L detection limits. A capillary column GS-Q was used on a Gas Chromatograph Trace Ultra (Thermo Electron Corporation) equipped with a FID detector. The samples were collected from Black See, situated at depth between 300 and 1400 m. **Acknowledgment.** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI – UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0178/ 24PCCDI/2018, within PNCDI III.

Poster T1-22

Analysis of the isotopic composition of the deep-sea sediments from the Black Sea

V Nagavciuc[1,2], R H Puscas [1], G Cristea [1], C Voica [1], S Radu [1], D A Magdas [1], G Ion[3] and I Turcu [1]

[1]National Institute for R&D of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]Faculty of Forestry, Ștefan cel Mare University of Suceava, Universitatii 12, 720229 Suceava, Romania

[3]National Institute for R&D of Marine Geology and Geoecology, 23-35 D. Onciul, 024053 Bucuresti, Romania

E-mail: nagavciuc.viorica@gmail.com

Abstract. The aim of this study is to analyse the deep-sea sediments from the Black Sea, using the stable isotopic and elemental content. For this purpose, 50 sediments samples were taken from five cores, having lengths between 2.66 and 4.24 m using the gravitational core. Additional ten samples were taken from three cores using the multicore equipment. All samples were collected during the marine expedition, on September 3-14, 2018, from the western part of the Black Sea. We determined δ13C and δ18O values and elemental concentrations (macro-elements, heavy metals) in sediments samples, along with δ18O and δ2H in extracted water from sediments. Preliminary results show that δ13C values range between -27.9 and -22.3 ‰ with a mean value of -25.3 ‰, while the δ18O values range between 0.5 and 10.2‰ with a mean of 4.6 ‰ from the sediments. In the extracted water, δ18O variation range was between -3.5 and 1.6 ‰, with a mean of -1.7 ‰, while δ2H values range between -32.4 and -16.5 ‰ with a mean of -23.1 ‰. The results of this research will be the basis of the new paleoclimatic reconstruction using stable isotopes in the deep-sea sediments from the Black Sea. Acknowledgment. This work was supported by a grant of the Romanian Ministery of Research and Innovation, CCCDI – UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0178/ 24PCCDI /2018, within PNCDI III.

Poster T1-23

Changes in composition and ultrastructure of green leafy vegetables after exposure to non-steroidal anti-inflammatory drugs

O Opriş[1], A Ciorîţă[1], M L Soran[1], I Lung[1] and L Copolovici[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]Faculty of Food Engineering, Tourism and Environmental Protection and Institute ofResearch, Innovation and Development in Technical and Natural Sciences of "Aurel Vlaicu" University, 2 Elena Drăgoi, 310330 Arad, Romania

E-mail: ocsana.opris@itim-cj.ro

Abstract. The aim of work was to assess the influence of the three most frequently used non-steroidal anti-inflammatory drugs (NSAIDs) of realistic environment concentrations on the autochthonous green leafy vegetables: orache (*Atriplex patula* L.) and spinach (*Spinacia oleracea* L.). Thus, chlorophylls, carotenoids and total polyphenol content were investigated and the ultrastructure of the leaves was evaluated when the green leafy vegetables were exposed to abiotic stress induced by NSAIDs (diclofenac, ibuprofen and naproxen). The results indicate a moderate reduction of chlorophylls, carotenoids and total polyphenol content. The investigations by transmission electron microscopy demonstrated that the green leafy vegetableswere affected by the selected NSAIDs. In general, ibuprofen affected the most of the green leafy vegetables. These results help us to better estimate the impact of drugs on environment and the importance of their responsible use.

Poster T1-24

Investigation of volatile and semi-volatile organic compounds profile of wines by SPME-GCxGC-TOFMS

D I Popescu, R E Ionete, C Ciucure and O R Botoran

National Research and Development Institute for Cryogenics and Isotopic Technologies – ICSI Rm. Valcea, 4 Uzinei Street, 240050 Rm. Valcea, Valcea, Romania

E-mail: diana.stegarus@icsi.ro

Abstract. Application of Solid Phase Micro-extraction (SPME) coupled with comprehensive two-dimensional gas chromatography with Time-of-Flight Mass Spectrometry (GCxGC-TOF MS) was used as alternative tool for characterisation of wines in terms of their volatile profile. Compared to the conventional one-dimensional GC, the GCxGC technique may provide significant improvement of compounds separation. The suitability of Headspace (HS) and Direct-Immersion (DI) sampling was also tested. The main goal of the work was to observe the differences between the qualitatively and semi-quantitatively analysis results of volatile compound classes in the wine samples, in the aim to assess the modification of the wine "bouquet" during aging (5 consecutively years, from 2015 to 2018). GCxGC chromatograms, compound list, peaks grouping with "Classification" software for major compound classes following by custom generated reports using "Compare" function applied on all organic compound classes grouped with "Classification" software, were also presented.

Poster T1-25

The correlation of the δ^2H-$\delta^{18}O$ values from atmospheric humidity with local rainfall Cluj-Napoca, Romania, between 2010-2011

R Puscas

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: rpuscas@itim-cj.ro

Abstract. Within the water cycle, temperature at the location where vapour condenses to precipitation has been heralded as a primary controlling factor in the fractionation of stable isotope in precipitation. Because atmospheric temperature dictates the pressure of aqueous vapour in atmosphere and water vapour pressure controls the isotopic composition of atmospheric water vapour, changes in temperature dictate different rates of fractionation.
This study was focused on the analysis and correlation of isotopic compositions of hydrogen and oxygen-18 in samples from atmospheric humidity with local rainfall. The isotope analysis of air moisture can greatly support in tracking the hydrological cycle through fingerprinting the source of water vapour, its transport and its condensation through direct analysis. This can be further used to understand factors controlling the water and energy balance of the atmosphere and guide new studies of clouds and the atmospheric hydrology. Time series for δ^2H and $\delta^{18}O$ values point out both the seasonal variation that has increased amplitude reflecting the continental character of the local climate as well as dramatic variations of isotopic content of successive precipitation events, emphasizing the anomalous values. **Acknowledgment**: The financial support for this work was provided by the Ministry of Research and Innovation, program Nucleu, contract no. PN 19 35 02 02.

Poster T1-26

Commissioning of a cryogenic distillation cascade for separation of carbon stable isotopes

Ş Bugeac[1], J Zs Szücs-Balázs[1], C M Varodi[1], C Lar[1], M C Marcu[1], A C Balla[1] and M L Gligan[1]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: zsolt.szucs@itim-cj.ro

Abstract. A carbon stable isotopes experimental separation plant was used at National Institute for Research and Development of Isotopic and Molecular Technologies from Cluj-Napoca, for high-level enrichment of carbon-13 by carbon monoxide cryogenic distillation. The experimental distillation plant consists of three parallel, 7 meter high packed separation columns, each of them equipped with adequate boiler and condenser. For the plant operation, a proper monitoring and control system was developed. The performance of the separation cascade was determined in production conditions, using different feeding points and different feedstockisotopic concentrations. Using the experimental results, the height of the theoretical plate, the separation for each columnand the overall separation was determined.

Poster T1-27

New weighted linear regression methods based on various weighting factors

V Taciuc[1] and A-C Moț[1,2]

[1]Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemistry, 11 Arany János, 400028, Cluj-Napoca, Romania

[2]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donath, 400293 Cluj-Napoca, Romania

E-mail: taciuc.vicentiu@gmail.com

Abstract. The effect of different weighting factors on the linear regression functions in the cases of heteroscedasticity are described and compared with ordinary and common weighted least squares methods. Applications of these new weighted methods to relevant experimental data sets demonstrated that the performance of the procedures proposed and efficiently applied in this comprehensive study exceed that of the ordinary least squares method and equals or often exceeds that of common weighted methods, using the inverse of variance ($1/s^2$) as a weighting factor. Applying various regression quality indices (coefficient of determination, standard deviation of estimate, quality coefficient of fittings), it was clearly proved that the following weighting factors (1/x, 1/residual, 1/d) are the most efficient.

Poster T1-28

Distribution of lithium content in Romanian foods using ICP-MS technique

C Voica[1], I Feher[1], D A Magdas[1], G Cristea[1]and A M Iordache[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] National Research and Development Institute for Cryogenics and Isotopes Technologies, 4 Uzinei, 240050, Ramnicu Valcea

E-mail: cezara.voica@itim-cj.ro

Abstract. Lithium is a naturally occurring alkali metal, naturally found in vegetables, grains and drinking water. Due to the nutritional studies, lithium is an essential trace element with a recommended dietary allowance of 1 mg/day. Lithium is used in therapeutic doses for treatment of depressive episodes. The natural lithium intake doses are much lower than those used for the treatment of patients with psychiatric disorders, but even very low lithium levels induced by routine consumption of lithium from water and food may have anti-suicidal effects. Some foods, though, can naturally increase the intake of the metal to levels that are unlikely to cause negative side effects. Over 200 food samples from Romanian marketwere analysed, from which 130 of basic food (oils, meat, milk and cheese samples) and the rest of vegetables samples. The lithium concentration was determined by ICP-MS technique and chemometric methods were used for results interpretation. Vegetables samples had the highest lithium content, followed by milk, cheese, meat and oil samples. Linear discriminant analysis (LDA) was applied separately on dairy products and vegetables in order to find the best markers that could differentiate the above-mentioned categories. **Acknowledgment:** The financial support for this work was provided by the Ministry of Research and Innovation**,** program Nucleu, contract no. PN 19 35 02 02.

Poster T1-29

Come old Briggs-Rauscher reaction – upgrades to an analytical tool

C Zăgrean-Tuza[1], S Dorneanu[1] and A C Moț[1,2]

[1]Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, 11 Arany Janos, 400028 Cluj-Napoca, Romania

[2] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donath, 400293 Cluj-Napoca, Romania

E-mail: cezarazt7@gmail.com

Abstract. Briggs-Rauscher reaction is one of the very few known oscillating processes which have continuously flabbergasted scientists. Its incongruous behaviour of alternating dominant chemical species is in fact based on a collection of usual processes that allow transitions between iodine and iodide. Definitely a milestone to our understanding of far-from-equilibrium chemical processes, this reaction has also proved to be a very cogent analytical tool in determining the antioxidant capacity, due to the fact that some compounds can interfere by ceasing the oscillations for a period of time. The aim of this research is to explore this assay by using spectroelectrochemistry in ascertaining its figures of merit compared to other well-established similar methods. In doing so, standards of polyphenols and complex samples have been employed. The results will be discussed from a penetrating analytical perspective. **Ackowledgement.** Financial support from Babes-Bolyai University (2018-2019 special scholarship for scientific activity 36.052/28.11.2018 to CZT) is gratefully acknowledged.

Section T2:

Molecules, Biomolecules and Green Technologies

Oral T2-1

Structural stability of Ni (II)-based macrocyclic-ligand complexes with square-pyramidal and octahedral coordination configuration

A Bende and A-A Farcaș

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: attila.bende@itim-cj.ro

Abstract. Intersystem crossings in different Ni(II) macrocyclic ligand complexes with square-pyramidal and octahedral ligand-metal coordination have been investigated by means of static (DFT) and time-dependent density functional theory (TD-DFT) calculations.Accordingly, two different, porphyrin- and diketo-pyrphyrin-based four-coordination macrocycles as planar ligand as well as pyridine and mesylate anion molecular groups as vertical ligands were considered in order to build the square-pyramidal and octahedral coordination configurations. For each molecular system the identification of equilibrium geometries and the intersystem crossing (the minimum energy crossing point) between the potential energy surfaces of the singlet and triplet spin states is followed by computing the spin-orbit couplings between the two spin states. Structures, based on the diketo-pyrphyrin macrocycle as planar ligand, show stronger five- and six-coordination organometallic complexes due to the extra electrostatic interaction between the positively charged central metal cation and the negatively charged vertical ligands. The results also show that the magnitude of the spin-orbit coupling is strongly influenced by the atomic positions of deprotonations of the ligands and implicitly the direction of the charge transfer between the ligand and the central metal ion.

Oral T2-2

DNA-Polyethyleneimine complex formation: coarse-grain simulations

T A Beu

Department of Biomolecular Physics, Faculty of Physics, University Babeș-Bolyai, 1 Mihail Kogălniceanu, Cluj-Napoca, 400084, Romania

E-mail: titus.beu@phys.ubbcluj.ro

Abstract. Due to the important medical implications, condensation of DNA-polycation complexes is a topicalmechanism related to gene-delivery. Given the high complexity of the biomolecular systems involved, realistic computational modelling is an essential aid in designing efficient DNA-polycation condensation set-ups. The remarkable buffering capacity, doubled by a relatively simple fabrication, make polyethyleneimine (PEI) a widely used gene-delivery vector. By employing Boltzmann inversion techniques, we derived from atomistic trajectories the coarse-grained (CG) parameters for a MARTINI-type force field (FF) for PEI. We performed extensive molecular dynamics simulations of DNA-PEI polyplex formation, making use of the developed FF for PEI and the standard MARTINI FF for DNA. We report a detailed analysis of the complexphenomenology involved, focusing on distributions of distances between the positive sites of the PEI and the negative phosphate groups of DNA. Our results demonstrate the crucial role of the PEI chain features in condensing DNA, expectedly being relevant for designing effective drug-delivery applications via the condensation phenomenon of DNA-PEI complexes.

Oral T2-3

DFT as support for experiment: The case of on-surface host-guest self assembly

L Buimaga-Iarinca and C Morari

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail:luiza.iarinca@itim-cj.ro; cristian.morari@itim-cj.ro

Abstract. Controllable host-guest systems are ones of the most interesting systems to date in nanotechnology. When, in addition, their interaction occurs on surface, these systems become even more interesting for practical applications. In this respect we have investigated by means of Density Functional Theory the controlled adsorption of small flexible molecules inside self-assembled pores that are formed on Cu(111) surface, as theoretical support for experimental scanning tunnelling microscopy data. Host isa highly ordered Cu-coordinated 4,9-diaminoperylene quinone-3,10-diimine (3deh-DPDI) porous network, while guest molecules are n-cycloalkenes (n=5 to 8).According to our model, it can be argued that all molecules prefer the region with negative potential (i.e. close to the pore-metal interface). Once a guest molecule is adsorbed, the electrostatic potential around it becomes even more negative. This suggests that the adsorption of a molecule inside the pore is creating a preferential adsorption zone for other molecules. **Acknowledgements**: Experimental data is provided by Nanolab team from UniBasel, Switzerland. The computational work was founded by the UEFISCDI, project PN-III-P4-IDPCE-2016-0217.

Oral T2-4

Structural insights into bacterial flagella

P Bulieris[1,2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donath, 400293 Cluj-Napoca, Romania

[2] Okinawa Institute of Science and Technology, 1919-1 Tancha, Onna-son, Okinawa, 904-0495, Japan

E-mail: paula.bulieris@itim-cj.ro

Abstract. Many bacteria use flagella to swim. The flagellum has a rotating motor located in the cell andan extra-cellular component that is formed of the rod, the hook and the filament. The filament functions as a helical propeller and the hook as a flexible universal joint. Two proteins, FlgK and FlgL, assure a smooth connectivity between the hook and the filament. The 3D structure of a major fragment of FlgK from *Campylobacter jejuni* was solved using X-ray crystallography. The structure of FlgK reveals that the cell-proximal half of the protein, is structurally conserved when compared with other known FlgK protein structures. However, the cell-distal half of the protein has diverged, developing a different 3D structure. Docking the model of the FlgK junction onto the structure of the*Campylobacter* hook provides significant clues about thisstructural divergence. My data show how evolutionary pressure to adapt to the structural constraints of *Campylobacter* flagella, causes divergence of one element of a supra-molecular complex in order to maintain the function of the entire flagellar assembly.

Oral T2-5

Strong impact of the orientation of transition dipole moments on the dynamics of diatomics in laser fields

P Badankó[1], G J Halász[1], L S Cederbaum[2], Á Vibók[1] and A Csehi[1]

[1]University of Debrecen

[2] University of Heidelberg

E-mail: csehi.andras@science.unideb.hu

Abstract. The formation of light-induced conical intersections (LICIs) between electronic states of diatomic molecules has been thoroughly investigated over the past decade. In the case of running laser waves, the rotational, vibrational, and electronic motions couple via the LICI giving rise to strong nonadiabatic phenomena. In contrast to natural conical intersections (CIs) which are given by nature and hard to manipulate, the characteristics of LICIs are easily modified by the parameters of the laser field. The internuclear position of the created LICI is determined by the laser energy, while the angular position is given by the orientation of the transition dipole moment (TDM) with respect to the molecular axis. In the present work, using MgH^+ as a showcase example, we exploit the strong impact of the orientation of the TDMs exerted on the light-induced nonadiabatic dynamics. Comparing the photodissociations induced by parallel or perpendicular transitions, a clear signature of the created LICIs is revealed in the angular distribution of the photofragments.

Oral T2-6

Principal Component Analysis used in medical data assessment

R Fechete[1,2], I A Morar[2,3], R E Dávid[3], R Pintican[4], R I Chelcea[1], D Moldovan[1] and A V Bumbu[5]

[1]Technical University of Cluj-Napoca, 103-105Muncii, 400641, Cluj-Napoca, Romania

[2]Babeş-Bolyai University, Faculty of Physics, 1 Kogălniceanu, 400084, Cluj-Napoca, Romania

[3]IMOGEN, County Emergency Hospital, L. Pasteur, 400349, Cluj-Napoca, Romania

[4]University Hospital, 3-5 Clinicilor, 40006, Cluj-Napoca, Romania

[5]Emergency County Hospital Oradea, Plastic Surgery Department, 37 Republicii, 410167, Oradea, Romania

E-mail: rfechete@phys.utcluj.ro

Abstract. A correct diagnostic after an *in vivo* imagistic examination or a realistic assessment of tissue regeneration is essential for an efficient treatment of patients. In the last years, the advanced *in vivo* NMR imaging (MRI) and spectroscopy (MRS) and *in vitro* ^{1}H NMR relaxometry are combined with classic methods for a complete characterization of microscopic properties of organic tissues. Nevertheless, the relevance of each parameter to the final diagnostic and/or assessment of the healing stage it was hard to be quantified. The Principal Component Analysis (PCA) is a statistical method largely used in many domains such as economics, social science, geology and not on the last place in medical investigations. We apply the PCA method to the differentiation between various types of woman's uterine cancer (taking into consideration also the healthy characteristics) and to the assessment of Wistar Albino rat's peripheral nerve regeneration after injury and two types of suture, direct suture and silicone graft. For that, multiple parameters were combines such as: concentration of relevant metabolites (from ^{1}H MRS), the main relaxation time T_2 (from T_2 maps and ^{1}H NMR relaxometry), tissue's water content, electric conductivity.

Oral T2-7

Principle Component Analysis as a discrimination tool. A case study on microorganisms

A M R Gherman[1,2]**, V Chiș**[2]**and N E Dina**[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Faculty of Physics, Babeș-Bolyai University,1 Mihail Kogălniceanu, 400084 Cluj-Napoca, Romania

E-mail: raluca.gherman@itim-cj.ro

Abstract. Principle Component Analysis (PCA) is a useful discrimination tool when one has to deal with big datasets of distinct samples, characterized by a large number of variables. This might be the case of spectroscopic data, such as (Surface-Enhanced) Raman spectra, where each wavenumber of a spectrum is considered a variable. The "know-how" of PCA, together with the math behind it will be discussed. PCAs performed on databases consisted of SERS spectra registered on different microorganisms (fungi – *Candida* species, yeasts – *Aspergillus* and *Rhizomucor* species, and Gram-positive and negative bacteria) will be given as examples.

Oral T2-8

Photothermoelectric detection of phase transitions. Liquid versus solid thermoelectric sensors

C Tripon and D Dadarlat

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: carmen.tripon@itim-cj.ro

Abstract. The new introduced photothermoelectric calorimetry was used in order to detect first and second order phase transitions. The paper is a synthesis of the most recent results obtained on ferroelectric (TGS), magnetic (Cr_2O_3) and liquid thermoelectric (dodecanol+TBAN) materials. Liquid (dodecanol+TBAN) and solid (CuCrO2) thermoelectrics have been used as sensors. The phothermoelectric method proved to be a suitable technique for phase transition detection, both for first and second order phase transitions and also for the measurement of critical behaviour of static and dynamic thermal parameters. It was demonstrated that using liquid thermoelectric sensors more accurate results have been obtained. The main reason was the elimination of the coupling fluid between the solid sample and the liquid sensor. **Acknowledgments.** This work was financially supported by Romanian Ministry of Research and Innovation, through the Core Program (Program Nucleu), project nr. PN 19 35 02 01.

Oral T2-9

Classical and quantum field-dressed spectra of the sodium molecule

T Szidarovszky[1], M Pawlak[2], G J Halász[3], Á Vibók[4]

[1] Laboratory of Molecular Structure and Dynamics, Institute of Chemistry, Eötvös Loránd University and MTA-ELTE Complex Chemical Systems Research Group, H-1117 Budapest, Pázmány Péter sétány 1/A, Hungary

[2] Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

[3] Department of Information Technology, University of Debrecen, PO Box 400, H-4002 Debrecen, Hungary

[4] Department of Theoretical Physics, University of Debrecen, PO Box 400, H-4002 Debrecen, Hungary a

E-mail: vibok@phys.unideb.hu

Abstract. In classical laser fields with frequencies resonant with the electronic excitation in molecules, it is by now known that conical intersections are induced by the field and are called light-induced conical intersections LICIs). As optical cavities have become accessible their quantized modes could also lead to the appearance of LICIs. In the present work theoretical frameworks are formulated for the investigation of LICIs of diatomics in such a classical and quantum light circumstances. As an example, by employing a weak measuring pulse, the dressed state absorption spectra of the Na2 molecule are investigated both in a cavity and in an optical lattice.

Oral T2-10

Allosteric protein-protein interactions in kinase networks involved in tumorigenesis

T Szimler, E Graczer, D Gyorffy, B Vegh, A Szilagy, I Hajdy, M Vas and P Zavodszky

[1]Institute of Enzymology, Research Center for Natural Sciences, Hungarian Academy of Sciences, 2 Magyar tudosok, 1117 Budapest, Hungary

E-mail: zavodszky.peter@ttk.mta.hu

Abstract. The tumour suppressor protein RASSF1A is phosphorylated by Aurora A kinase, thereby impairing its tumour suppressor function. Consequently, inhibiting the interaction between Aurora A and RASSF1A may be used for anti-tumour therapy. We used recombinant variants of RASSF1A to map the sites of interaction with Aurora A. The phosphorylation kinetics of three truncated RASSF1A variants has been analysed. Compared to the RASSF1A form lacking the 120-residue long N-terminal part, the Km value of the phosphorylation is increased from 10 to 45 μM upon additional deletion of the C-terminal SARAH domain. On the other hand, deletion of the flexible loop (Δ177-197) that precedes the phosphorylation site/s (T202/S203) results in a reduction of the kcat value from about 40 to 7 min-1. Direct physical interaction between the isolated SARAH domain and Aurora A was revealed by SPR. These data demonstrate that the SARAH domain of RASSF1A is involved in the binding to Aurora A kinase after the formation of a new allosteric site, as a consequence of the RASSF1A RAS-binding domain and the AuroraA kinase domain interaction. Structural modelling confirms that such a novel complex is feasible between the SARAH domain and the kinase domain of Aurora A. In addition, a regulatory role of the loop in the catalytic phosphorylation reaction has been demonstrated both experimentally and by structural modelling. Our experiments and modelling suggest that the mechanism of this binding is a ligand induced conformational change, the less-structured ligand, the fuzzy SARAH-helix of the monomeric form of RASSF1A adapts to the target and the conformation of the SARAH domain is stabilized upon this binding.

Poster T2-1

Polyethyleneimine: coarse-grain modeling and simulations

A E Ailenei, R I Costinaș and T A Beu

Department of Biomolecular Physics, Faculty of Physics, University Babeş-Bolyai, 1 Mihail Kogălniceanu, Cluj-Napoca, 400084, Romania

E-mail: andradaailenei95@yahoo.com

Abstract. The computational design of realistic soft-matter systems presents a wide range of technical challenges due to the inherent complexity of biological molecules. Aiming to accurately model polyethyleneimine (PEI) as a drug delivery vector, we conducted extensive atomistic (AA) molecular dynamics simulations. In order to develop a coarse-grained (CG) force field (FF) for PEI we extractedfrom the AA trajectories the force constants and equilibrium values for the bonded interactionsby Boltzmann inversion. Moreover, we employed this new FF in CG simulations analysing the PEI behaviour in terms of gyration radius and end-to-end distance. The study was performed for standard versus polarizable CG water, and the long-range electrostatic interactions were treated comparatively with the Reaction Field-and Particle Mesh Ewald methods. In particular, polarizable water in conjunction with reaction-field electrostatics yields structural properties in good agreement with the AA analogues.

Poster T2-2

Study on the correlation of PAH's content in soil and air with the concentration of PAH's in leaves and flowers

V Băbălău-Fuss[1,2], M Roman[1], A Moldovan[1,3], A Becze[1]and M Tofană[2]

[1]INCDO-INOE2000, Research Institute for Analytical Instrumentation, ICIA Cluj-Napoca Subsidiary, 400293 Cluj-Napoca, Romania,

[2]University of Agricultural Sciences and Veterinary Medicine Cluj-Napoca, 400372 Cluj-Napoca, Romania

[3]Technical University, Faculty of Materials and Environmental Engineering, 103 - 105 Muncii Bulevard, 400641, Cluj-Napoca, Romania

E-mail: anca.naghiu@icia.ro

Abstract. PAH's are a group of hydrocarbons that countain two or more aromatic rings and are ubiquitous found in nature. The European Union regulates concentrations of PAHs in air, water, soil and food due to their carcinogenicity or genotoxicity properties. The aim of the study was to correlate the PAH's content in soil and air with the content in flowers from *Prunus spinosa* (blackthorn) and leaves from *Rosa canina* (dog rose). Samples of soil, air, leaves and flowers were taken in spring time from Cluj County area. Hexan was used for the extraction of samples and HPLC with FLD for analysis of naphthalene, acenaphthene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, benz[a]anthracene, chrysene, benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[a]pyrene, indeno[1,2,3,c,d]-pyrene, dibenz[a,h]anthracene and benzo[g,h,i]perylene. For the extraction of flowers and leaves an Accelerated Solvent Extraction (ASE) system was used. The average value of total PAH's found in the soil samples was 51,34 µg/kg. There was positive correlation between higher levels of PAH's found in air and the content of PHA's in leaves and flowers.

Poster T2-3

Short peptide shows efficacy against methicillin-resistant Staphylococcus aureus strains

M Bacalum[1], E C Dragulescu[2], I Codita[2,3] and M Radu[3]

[1]Department of Life and Environmental Physics, "Horia Hulubei" National Institute of Physics and Nuclear Engineering, Măgurele, Romania

[2] Nosocomial and Antimicrobial Resistant Infections Laboratory, "Cantacuzino" National Medico-Military Institute for Research and Development, Bucharest, Romania

[3] "Carol Davila" University of Medicine and Pharmacy, Bucharest, Romania

E-mail: bmihaela@nipne.ro

Abstract. In recent years methicillin-resistant Staphylococcus aureus has posed a challenge in treating skin and soft tissue infections. Finding new antimicrobial agents has therefore become imperative. We evaluated the in vitro antimicrobial activity of a synthetic peptide, P6, against multidrug resistant clinical strains of Staphylococcus aureus isolated from skin and soft tissue infections. The P6 antimicrobial effect was evaluated in vitro by determining MIC/MBC, the ratio of live/dead cells and the effects induced at membrane level. The therapeutic efficiency was determined against human skin cells. P6 inhibited growth for all strains between 8 and 16 mg/L and killed all bacterial strains at 16 mg/L. The therapeutic potential was found to be 30 and 15 in the presence of BSA. We showed that P6 localizes at membrane level, where it acts slowly, by depolarizing it and affecting its integrity. P6 can be considered a good candidate for use as an antimicrobial agent in topical applications.

Poster T2-4

The Study of Green Corrosion Inhibition on Carbon Steel Using Acidic Media

N Cotolan[1], D Bogdan[2] and J D Chelaru[1]

[1] Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemical Engineering, 11 Arany Janos, 400028 Cluj-Napoca, Romania

[2] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: diana.bogdan@itim-cj.ro

Abstract. Th e aim of the present work is to assess the feasibility of using the naturally occurring, inexpensive and eco-friendly inhibitor for the corrosion inhibition of carbon steel (C-steel) in acidic media. A set of electrochemical techniques were used in order to obtain and investigate the samples, as follows: Electrodeposition, Open Circuit Potential (OCP), Linear Polarization (LP), Tafel plots and Electrochemical Impedance Spectroscopy (EIS). Atomic Force Microscopy (AFM) has been used to investigate the surface characteristics, mainly the topography, of the unmodified and modified electrodes based on C-steel. The metal surface morphology and chemical characterization of green inhibitor were also investigated by various microscopy and spectroscopic techniques. **Acknowledgements**: NC and JDC are grateful for the financial support of the Romanian Ministry of Research and Innovation, CCCDI-UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0652/84PCCDI/2018, within PNCDI III. DB acknowledges financial support from the Romanian Ministry of Research and Innovation through the Core Program, Project PN19 35 02 01.

Poster T2-5

Crystal and molecular structure of cardarine

G Borodi[1], A Turza[1], S Albert[1] and P A Camarasan[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]Faculty of Environmental Science and Engineering, Babes-Bolyai University, 30 Fantanele, 400000 CLuj-Napoca, Romania

E-mail: borodi@itim-cj.ro

Abstract. The crystal structure of Cardarine, systematic name: {4-[({4-methyl-2-[4-(trifluoromethyl)phenyl]-1,3-thiazol-5-yl}methyl)sulfanyl]-2-methylphenoxy}acetic acid has been determined by X-ray single crystal diffraction. Cardarine is a PPARδ receptor agonist and was developed for treatment of cardiovascular disease, having also sport enhancing properties. The compound was found to crystallize in P 21/n space group of the monoclinic crystal system, having the following lattice parameters: a=10.92669(10)Å, b= 9.68349(11)Å, c= 19.7719(2)Å, $\alpha=90^0$ $\beta=98.2167(10)^0$ $\gamma=90^0$. The supramolecular stability is assured by O-H...N hydrogen bonding and a combination of C-H..O, O-H...C, C-H...C short contact intreactions. Hirshfeld analysis and lattice energy computation by Coulomb-London-Pauli method has been made in order to investigate the interactions within the crystal.

Poster T2-6

Nanoscale investigation of low generation PAMAM dendrimers

I Schiopu[1], I C Bucataru[2], T Luchian[3], C H Seo[4] and Y Park[5]

[1]Interdisciplinary Research Institute - Sciences, Alexandru Ioan Cuza University of Iasi, 700506, Romania

[2]Faculty of Physics, Alexandru Ioan Cuza University of Iasi, 700506, Romania

[3]Department of Physics, Alexandru Ioan Cuza University of Iasi, 700506, Romania

[4]Department of Bioinformatics, Kongju National University, Kongju 32588, South Korea

[5]Department of Biomedical Science and Research Center for Proteinaceous Materials (RCPM), Chosun University, Gwangju 61452, South Korea

E-mail: bucataru.cezara93@gmail.com

Abstract. Polyamidoamine (PAMAM) dendrimers are nano-sized molecules with applications in the biomedical field. Their main structural components are: the ethylenediamine core, the radially repeating amidoamine units and the terminal amino functional groups. Herein, we investigated the interactions between both openings of an α-hemolysin (α-HL) protein nanoporeand PAMAM dendrimers of different generations. The statistical analysis of the inter-events time, the dwell time and the blockade amplitude unveiled the distinct kinetics of the stochastic process of interaction between the α-HLand the PAMAM of low generation added from either side of the nanopore. **Acknowledgements***:* NRF-2016R1A2A1A05005440, GRL-NRF-2014K1A1A2064460, IITP-Grant-MSIT-2017-0-01714; PN-III-P4-ID-PCE-2016-0026, CCCDI-UEFISCDI; PN-III-P1-1.2-PCCDI-2017 0010/74/2018; 25/2018-PN-III-P1-1.1-PD-2016-0737.

Poster T2-7

Monitoring the degradation of packaging products by advanced ^{1}H NMR relaxometry, Vis-near IR and FT-IR spectroscopy

R I Chelcea, D Moldovan, F G Rus and R Fechete

Technical University of Cluj-Napoca, Physics and Chemistry Department, 28 Memorandumului, 400114, Cluj-Napoca, Romania

E-mail: Ramona.Chelcea@phys.utcluj.ro

Abstract. Since the appearance of modern food sold in supermarkets, the packaging innovation have been a major component of food industry. In recent years, there has been an increasing demand for bio-packaging, which offer additional to the ease of use and food safety an environmentally friendly way of waste disposal and/or recycling. As containers for food packing are used both plastic and paper, the emphasis being on biodegradable materials. We investigate such commercially available packing materials: corn starch, 100% biodegradable bag, paper, polyethylene, thermal insulation and household bags. To characterize their degradation the bags were subjected in natural conditions for 24 weeks to different types of aging factors such as: distilled water, hydrogen peroxide, natural degraded for the same period and to artificial UV-irradiation up to 30 minutes. The effect of degradation on packaging materials was investigated using ^{1}H NMR relaxometry correlated with advance data processing by the Laplace inversions, Vis-nearIR and FT-IR spectroscopy. Even at one week of degradation the dynamic properties of the bags are substantially changed. The most severe degradation was suffered by the corn starch bag, while the least degraded was the thermal insulation bag. The paper bag was almost totally dissolved in distilled and oxygenated water.

Poster T2-8

Designing, building and monitoring of a laboratory scale modular green roof model

R Crainic and R Fechete

Technical University of Cluj-Napoca, Faculty of Material and Environmental Engineering, 103-105Muncii, 400641, Cluj-Napoca, Romania

E-mail: ramona.crainic95@gmail.com

Abstract. Nowadays solutions of green roofs appeal as a smart way of adding green infrastructure to a crowded city since they can be included on new buildings or onto existing buildings, and require little space at ground level. Benefits of a green roof are multiple such as: i) stormwater retention to reduce peak flow and runoff; ii) water quality enhancement for water utilization; iii) to improve the environmental and reduce energy cost; iv) air cleaning for easy comfort into crowded urban areas; v) noise level reduction; vi) ecological benefits by enhancing the aesthetic of an area; vii) social and economic benefits. We design and build a laboratory scale model of a modular green roof. The main layers of each modulus are water proofing membrane, root barrier membrane, drainage layer, filter layer, vegetation. Modulus 1 will have a regular growth medium and modulus 2 will have a grown medium with volcanic ashes. The model will be online monitored via a series of smart sensors like soil humidity and temperature, radiation level (infrared, visible and ultraviolet), air humidity and temperature. A seismic alert it is also implemented. The soil and stormwater are characterized by pH, electric conductivity, turbidity, ^{1}H NMR relaxometry and diffusometry.

Poster T2-9

Thermal inspection of royal jelly. Photopyroelectric approach.

R Margaoan[1], C Tripon[2], O Bobis[3], V Bonta[3] and D Dadarlat[2]

[1]Advanced Horticultural Research Institute of Transylvania, USAMV, 400372 Cluj-Napoca, Romania

[2] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[3]Life Science Institute "King Michael I of Romania", USAMV, 400372 Cluj-Napoca, Romania

E-mail: dadarlat@itim-cj.ro

Abstract. Fifteen samples of royal jelly delivered by different producers have been investigated by photopyroelectric (PPE) calorimetry. The thermal diffusivity was obtained in the back PPE configuration, by performing a sample's thickness scan of the phase of the PPE signal. In order to obtain the thermal effusivity, a frequency scan of the phase of the PPE signal was performed, in the front PPE detection. The remaining two thermal parameters, thermal conductivity and volume specific heat were calculated using classical relationships. As a result, similar values for all static and dynamic thermal parameters have been found. Additional phase transitions investigations have been performed in the front PPE configuration, in the -17 ^{0}C ÷ 8 ^{0}C temperature range. The results are split: some samples presented only one first order (solid/liquid) phase transition, but other are involved in two phase transitions indicating a coexistence of two different phases. In conclusion, the PPE method, used in a temperature scan arrangement, can offer structural information about this type of samples. In addition, chemical analysis supports the PPE results.

Poster T2-10

Clusters tagged by alkali metals

T M Di Palma[1], **M F Gaele**[1] **and A Bende**[2]

[1]Consiglio Nazionale delle Ricerche, Istituto Motori, 8 Via Marconi, 80125 Napoli, Italy

[2]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: t.dipalma@im.cnr.it

Abstract. Water clusters and Mixed Formic acid-water clusters produced in molecular beam have been tagged by one sodium atom and investigated by mass spectrometry and tunable UV laser photoionization. Two series of clusters Na-$(H_2O)_n$ and Na-$(HCOOH)(H_2O)_n$ have been detected at various photon energies, from their appearance threshold in the mass spectrum up to 0.5 eV above. The appearance energies of the mixed clusters, as a function of cluster size, show a flattening shifted toward higher energies with respect the pure water cluster. This spectroscopic signature is indicative of a significant contribute from the acid molecule to the water cluster and may be useful to predict more carefully the structure of ionized and neutral clusters.

Poster T2-11

Advanced characterization of plastering mortars with glass waste additives

L R Drăgan[1], **E Jumate**[2], **C Aciu**[2], **D L Manea**[2] **and R Fechete**[1,3]

[1] Technical University of Cluj-Napoca, Faculty of Material and Environmental Engineering, 103-105Muncii, 400641, Cluj-Napoca, Romania

[2] Technical University of Cluj-Napoca, Faculty of Civil Engineering, 25 Baritiu, 400027, Cluj-Napoca, Romania

[3] Babeş-Bolyai University, Faculty of Physics, 1 Kogălniceanu, 400084, Cluj-Napoca, Romania

E-mail: laviniadragann@yahoo.com

Abstract. As result of modern medical treatments, worldwide an immense quantity of glass waste is produced. The main waste originates in the remaining glass medicine containers. Instead of throwing away as garbage, we propose to recycle the empty glass contains as replacement of aggregates, especially sand, from plastering mortars. Several formulations of plastering mortars without and with glass of variable granulation, without and with antibiotic drugs was prepared. For each formulation seven prisms were casts. Pairs of two prisms were tested at 3, 7 and 28 days after preparation by measuring the mechanical resistance at elongation and compression. In the seventh prism a pair of humidity and temperature sensors was placed in order to monitor the hydration and dehydration processes to characterize the effect of aggregates replacement by glass waste. Advanced ^{1}H NMR relaxometry and diffusometry measurement were performed on samples parts resulted from mechanical tests at 3, 7 and 28 days after preparation. Then the samples were sunken in water and measured again after a full hydration of plaster mortar stone. The experimental data were analysed by inverse Laplace transform and the distributions of transverse relaxation time T_2 and self-diffusion coefficient D were obtained. The possible antibiotic effect was evaluated.

Poster T2-12

Interaction of tumor-homing peptides with lipid membranes

I S Dragomir[1], **C Ciobănașu**[2], **A Apetrei**[1] **and T Luchian**[1]

[1]Department of Physics, Alexandru I. Cuza University, 700506 Iasi, Romania

[2]Interdisciplinary Research Institute, Sciences Department, Alexandru I. Cuza University, 700506 Iasi, Romania

E-mail: isdragomir@yahoo.ro

Abstract. Accounting 9 million deaths annually, cancer still represents a major challenge for scientific community. Discovery of new peptides with high penetration ability of plasma membrane and specificity for receptors overexpressed in tumors, is of particular interest in the development of new drug delivery systems. These peptides, called tumor-homing peptides, are the best candidates for specific and high efficiency delivery of imaging and therapeutic agents and other molecules of interest. Lyp-1, a cyclic 9-amino-acid peptide is a homing peptide that specifically binds to tumor-associated lymphatic vessels, breast carcinoma, osteosarcoma and prostate carcinoma. Linear tLyp-1shows specificity for breast cancer, tumor vasculature, prostate carcinoma and glioma. In this work we investigated the interaction between fluorescently labelled Lyp-1 and tLyp-1 with model membranes, called Giant Unilamellar Vesicles (GUVs) using confocal fluorescence microscopy. Our experimental results revealed that Lyp-1 and tLyp-1 translocate across the GUVs membranes of different lipid composition suggesting that these peptides have also a passive, energy-independent internalization mechanism. **Acknowledgement**: Grant of the Romanian Ministry of Research and Innovation, CCCDI-UEFISCDI, project no. 74PCCDI/2018, code PN-III-P1-1.2-PCCDI-2017-0010, within PNCDI III.

Poster T2-13

Nanoscopic investigation of hydrophilic and hydrophobic amino acids-containing peptides interaction with the α-HL nanopore

I S Dragomir[1], A Asandei[2], I C Bucătaru[1], G Di Muccio[3], M Chinappi[3], Y Park[3] and T Luchian[1]

[1] Department of Physics, Al I Cuza University, 700506 Iasi, Romania

[2] Interdisciplinary Research Institute, Sciences Department, Al I Cuza University, 700506 Iasi, Romania

[3] Department of Industrial Engineering, University of Rome Tor Vergata, Via del Politecnico 1, 00133 Rome, Italy [4] Department of Biomedical Science and Research Center for Proteinaceous Materials, Chosun University, 61452 Gwangju, Korea

E-mail: isdragomir@yahoo.ro

Abstract. Single-molecule electrophysiology techniques probing the interaction between distinct molecules and protein nanopores inserted into artificial lipid bilayers, unravel insights about the identity and physico-chemical properties of the studied analytes. Herein we studied the paradigm of real-time discrimination of groups of hydrophilic and hydrophobic amino acids present on the primary structure of custom-engineered peptides, flanked by segments of oppositely charged amino acids, enabling peptide slowdown across the nanopore. We offer evidence supporting the possibility of discriminating between patches of hydrophilic and hydrophobic amino acids, by quantifying the relative blockade exerted by the peptides on the ionic current through the nanopore, and the transit times of peptides across the nanopore. **Acknowledgements:** The authors acknowledge the financial support offered by grants PN-III-P4-ID-PCE-2016-0026 (NANOTWEEZ-TL), PN-III-P1-1.1- TE-2016-0508 (PEPREC - AA), PN-III-P1-1.2-PCCDI-2017-0010 (TehnoBioMed-TL) and Global Research Laboratory (GRL) Grant (NRF-2014K1A1A2064460).

Poster T2-14

Surface enhanced Raman spectroscopy (SERS) investigations of saliva for oral cancer diagnosis

A Falamas[1] and M Hedesiu[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Department of Oral Radiology, "Iuliu-Hateganu" University of Medicine and Pharmacy, Cluj-Napoca, Romania

E-mail: afalamas@itim-cj.ro

Abstract. Recently, saliva has been considered as a possible diagnosis tool, due to its collection advantages and its composition, which can reflect the health status of an individual. The numerous proteins it contains can be used as biomarkers for disease diagnosis when high-sensitive detection techniques are employed. In this study we explore the enhancement of salivary characteristic Raman bands by using label-free, ultrasensitive surface enhanced Raman spectroscopy (SERS). The aim of the study is to investigate the possibility of using the molecular vibrational information obtained from saliva samples for oral cancerdiagnosis. Saliva was collected in the morning from both healthy and cancerous patients, kept at -80^{o}C, and centrifuged at 9000g for 20 min to remove oral impurities. The supernatant was mixed with Au colloidal nanoparticles and SERS spectra were collected from dried spots pipetted on glass slides, following excitation at 785 nm. A continuous on and off SERS blinking was observed when time series spectra were collected from various locations on the samples. Preliminary measurements and multivariate analyses will be presented. This work was supported by a grant of the CNCS-UEFISCDI, project number PN-III-P1-1.1-PD-2016-1057.

Poster T2-15

Light induced singlet-triplet transition in metal-ligand coordination complexes

A A Farcaş[1,2], T A Beu[2] and A Bende[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Babes-Bolyai University, Faculty of physics, 1Mihail Kogălniceanu, 400084Cluj-Napoca, Romania

E-mail: alexfadrian@yahoo.com

Abstract. Light induced singlet-triplet transition for Ni(II)-based macrocyclic-ligand complexes: Ni–tetrakis(pentafluorophenyl)porphyrin functionalized with a single phenazopyridine arm (NiTPP-PAPy) and Ni(II)–tetrakis-porphyrin functionalized with two phenazopyridine arms (NiTP-biPAPy) have been investigating using time-dependent density functional theory. The calculations have been performed using the MN12-SX exchange correlation functional combined with the def2-TZVP basis set. The singlet-triplet spin transitions have been characterized by searching for the intersystem crossing (ISC) point between the two potential energy surfaces of the ground state singlet and triplet spin states. The strength of the spin-orbit coupling for the ISC geometry was also computed. The active electronic excited states involved in the light induced spin transitions were identified both for singlet and triplet excited electronic states. The presence of the moderate high barriers defined bythe minimum energy crossing points between the singlet and triplet equilibrium geometries of the NiTPP-PAPy and NiTP-biPAPy supramolecular complexes might be able to prevent the thermal-driven spin transition and thus facilitates the light-induced spin flip.

Poster T2-16

Simple models that mimic the lipid composition in the mammalian and bacterial membranes

A Farcaş[1] and L Janosi[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: alexandra.farcas@itim-cj.ro

Abstract. Antimicrobial drug resistance is one of the major threats to global public health today. The growing interest in natural antimicrobial peptide (AMP)-based therapeutics is intimately related to antibiotic resistance. Because the AMPs present a high selectivity between bacterial and eukaryotic cells, their mode of action in model membranes is essentially. Therefore, we modelled these membranes as bilayers with different lipid compositions. In order to realistically reproduce the cell properties, we studied both simple and complex lipid bilayers by employing atomistic and coarse-grained molecular dynamics simulations. We characterized the mammalian and bacterial models and we compared various parameters like thickness, number density, lipid tilt angle and order parameter. Hence, in the present study, we propose different membrane models, which are needed to identify peptides with low cytotoxicity against mammalian membranes, as well as high antimicrobial activity against bacterial membranes. **Acknowledgement:** This work was supported by a grant of Ministry of Research and Innovation, CNCS – UEFISCDI, project number PN-III-P1-1.1-TE-2016-0032.

Poster T2-17

Toxicological evaluation of graphene-based nanoparticles on epithelial cells

A Farcaș[1,2], M Suciu[1,2], V Toma[1,2], M C Corobea[3] and I Turcu[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Babes-Bolyai University, Faculty of Biology and Geology, Cluj-Napoca, Romania

[3] National Institute for Research and Development in Chemistry and Petrochemistry-ICECHIM, Department of Polymers, Bucharest, Romania

E-mail: farcas.anca14@itim-cj.ro

Abstract. Understanding the behaviour of epithelial cells when interacting with graphene-based materials is a key strategy to the development of several technologies and of the management of graphene health and safety issues. Exposing epidermal human keratinocytes (HaCaT) and fibroblasts (BJ) to commercially available graphene nanoplatelets (GNP), such as C500 and M5, do not lead to any morphological changes. The cell viability status was assessed using the MTT assay which was useful to establish the optimal concentration for the further experiments. The intracellular oxidative status was measured throughout enzymatic and non-enzymatic antioxidants, such as catalase (CAT) activity, superoxide dismutase (SOD) activity and glutathione concentration (GSH). Hence, these biochemical indicators revealed non-significant changes of the oxidative status. *Summa summarum*, graphene-based nanoparticles C500 and M5 do not have an aggressive or toxic effect upon human epithelial HaCat and BJ cells.
Acknowledgements: This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI – UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0387 / 80PCCDI/2018, within PNCDI III.

Poster T2-18

NMR investigation of an inverse freezing counterintuitive phenomenon

C G Floare[1], A Pîrnău[1], C Filip[1], I Ardelean[2] and M Bogdan[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]Technical University Cluj Napoca, Department of Physics & Chemistry, Cluj Napoca 400258, Romania.

E-mail: calin.floare@itim-cj.ro

Abstract. Our surprising discovery of a system which solidifies under heating and melts when the temperature decreases has attracted much interest and has been intensively studied using neutron scattering experiments and high-resolution powder diffraction measurements at ILL and ESRF, Grenoble, France. This unusual behavior has been also characterized by differential scanning calorimetry and solubility measurements, proving that it is caused by an extraordinarily strong negative temperature coefficient of the solubility of αCD in the mixture of 4MP and a small quantity of water, water playing a crucial role in the solidification process. This contribution is a review of the results obtained until now on the investigation of this peculiar effect and we also present our recent results using proton NMR relaxation technique. **Acknowledgements.** This work was financially supported by Ministry of Research and Innovation, Romania, through the Core Program, Project PN 19 35 02 01 and in its initial stage by Project CEEX ET-58/2006.

Poster T2-19

Molecular affinity analysis of levo-thyroxine on BSA modified gold chip using molecular scale methodologies

M David[1], C Chilom[2] and M Florescu[1]

[1] Transilvania University of Brasov, Faculty of Medicine, 29Eroilor, 500036 Brasov, Romania

[2] University of Bucharest, Faculty of Physics,405 Atomistilor, 077125 Magurele, Romania

E-mail: florescum@unitbv.ro

Abstract. Levo-thyroxine hormone (LT4) plays an important role in the human organism, being linked to several medical conditions such as hypothyroidism. In this work, we monitor the binding mechanism of LT4 directly to bovine serum albumin (BSA) molecules, free into solution and confined to a gold chip. Using the fluorescence emission properties of the two tryptophan residues in BSA, the BSA quenching mechanism of LT4 was characterized. The T4-BSA binding was followed by the affinity constant, showing the strength of the interaction and by thermodynamic parameters, which put in evidence the driving forces involved in binding of LT4 to BSA site.Surface plasmon resonance (SPR) and electrochemical impedance spectroscopy (EIS) were used to monitorthe interfacial changes occurring at the surface of BSA modified gold coated chip and so study the affinity and kinetics of biomolecular interactions between LT4andBSA confined to a gold chip. **Acknowledgments.** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0062, contract no. 58, within PNCDI III. We hereby acknowledge the structural founds project PRO-DD (POS-CCE, O.2.2.1., ID 123, SMIS 2637, No 11/2009) for providing the infrastructure used in this work.

Poster T2-20

Al-air batteries with solid hydrogel electrolytes: effect of pH on cell performance and rechargeability

T M Di Palma, F Migliardini, M F Gaele and P Corbo

Consiglio Nazionale delle Ricerche, Istituto Motori, 8 Via Marconi, 80125 Napoli, Italy

E-mail: t.dipalma@im.cnr.it

Abstract. Metal-air batteries are very promising sources of energy for various applications, such as electronics, electric vehicles and smart grid energy storage. The most important feature of a metal-air battery is the coupling of a metal anode, characterized by a high energy density, and a catalysed cathode with an open structure capable of continuously aspirating and reducing oxygen from the atmosphere. This characteristic is responsible for the theoretically high energy density, generally associated with this type of device. The use of Al anodes in metal-air galvanic cells is particularly interesting due to its intrinsic physico-chemical properties: high theoretical specific capacity (2.98 Ah g-1) comparable to that of Li (3.86 Ah g- 1) light, negative standard potential vs. SHE, abundance in the earth's crust, recyclability and environmental friendliness. In this paper different hydrogels based on xanthan have been prepared at different pH values in order to obtain solid electrolytes characterized by high ionic conductivity. These electrolytes have been tested in Al-air galvanic cells using Pt/C based air cathodes. The performance of cells has been verified by discharge tests at constant currents in the range 1-10 mA/cm^2. The possibility to recharge the cells has been evaluated determining the electrolyte electrochemical window by cyclic voltammetry experiments. The different electrochemical parameters of cells have been determined by electrochemical impedance spectroscopy.

Poster T2-21

Halogen bonding directed supramolecular architectures of 2,7-dipyridylfluorene co-crystals

I G Grosu[1], L Pop[2], M Miclăuş[1], N D Hădade[2], A Terec[2] and I Grosu[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Babeş-Bolyai University, Department of Chemistry and CSOOMC, 11 Arany Janos,400028 Cluj-Napoca, Romania

E-mail: ioana.grosu@itim-cj.ro

Abstract. Halogen bonding is an emerging noncovalent interaction for constructing supramolecular complexes and networks. Together with other weak interamolecular interactions such as hydrogenbonding, π donor – acceptor contacts and hydrophobicity of the perfluorocarbons, halogen bonding can be used to design and synthesize appealing supramolecular architectures, opening new insights to materials design. In this context, we considered of interest to investigate the access, structures and properties of supramolecular architectures obtained from dipyridylarenes as halogen acceptors and diiodobenzene or diiodo-tetrafluorobenzene derivatives as halogen donors. Four supramolecular polymers were obtained by solvent assisted mechanochemical ball-milling method. The formation of the products was monitored by powder X-ray diffractometry and their crystal structures were determined by single-crystal X-ray diffraction. **Acknowledgements**: Financial support from the Ministry of Research and Innovation—MCI, Core Programme, Project PN19 35 02 01.

Poster T2-22

Amino acids - a major target for antioxidants

A Guidea, D Casoni, A C Moț and C Sârbu

Research Center for Advanced Chemical Analysis, Instrumentation and Chemometrics, Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, 400028, Cluj-Napoca, România

E-mail: aguidea@chem.ubbcluj.ro

Abstract. The search for effective, nontoxic natural compounds with antioxidative activity has been intensified in recent years. The present work provides a brief overview of protein-related amino acids as a natural antioxidant as a result of their abundance in biological systems. The antioxidant properties were studied using the following methods: the 2,2-di(4-tert-octylphenyl)-1-picrylhydrazyl (DPPH), 2,2'-azinobis-3-ethylbenzothiazoline-6-sulfonic acid (ABTS), superoxide radical scavenging activity (SORS), and nitric oxide (NO) radical scavenging methods along with cupric ion reducing antioxidant capacity (CUPRAC), chromium reducing antioxidant capacity (CHROMAC), ferric reducing antioxidant power (FRAP) and metal chelating activity method. Chemometric techniques such as cluster analysis (CA) and principal component analysis (PCA) and especially fuzzy clustering (FC), were used in order to classify the amino acids according to their antioxidant activity evaluated by applied experimental methods. The sum of ranking differences (SRD) analysis was used for ranking the performance (power of discrimination) of the methods in the determination of the same property. Results from the multivariate exploratory techniques revealed that the essential amino acids can be classified into high, medium and low antioxidants. The highest antioxidant amino acids (cysteine (non-essential amino acid) and tryptophan (essential amino acid)) were classified in the same group with the most antioxidant biogenic amines and related drugs. FC find out, in the better way, the (dis)similarity of amino acids within of each antioxidant scales. Based on SRD results, the method that best discriminates the amino acids is the DPPH radical scavenging method.

Poster T2-23

Ultrafast dynamics in the vicinity of quantum light-induced conical intersections

T Szidarovszky[1], G J Halász[2], A G Császár[1], L S Cederbaum[3] and Á Vibók[4]

[1] Laboratory of Molecular Structure and Dynamics, Institute of Chemistry, Eötvös Loránd University and MTA-ELTE Complex Chemical Systems Research Group, H-1117 Budapest, Pázmány Péter sétány 1/A, Hungary

[2] Department of Information Technology, University of Debrecen, PO Box 400, H-4002 Debrecen, Hungary

[3] Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, D-69120, Heidelberg, Germany

[2] Department of Theoretical Physics, University of Debrecen, PO Box 400, H-4002 Debrecen, Hungary a

E-mail: halasz@inf.unideb.hu

Abstract. As an alternative to interactions of atoms or molecules with intense laser fields, strong light-matter coupling can also be achieved, both for atoms and molecules, by their confinement in microscale optical or plasmonic cavities. A theoretical framework is formulated for investigating the rovibronic spectra of molecules coupled to one mode of the radiation field in an optical cavity. The approach involves the computation of cavity-field-dressed rovibronic states, which are hybrid light-matter eigenstates of the "molecule + cavity radiation field" system, and the computation of transition amplitudes between these field-dressed states with respect to a weak probe pulse. The cavity-field-dressed rovibronic spectrum of Na2 demonstrates undoubtedly the presence of a "light-induced conical intersection" induced by the quantized radiation field. Dependence of the cavity-field-dressed spectrum on the cavity-mode wavelength as well as on the light-matter coupling strength is investigated.

Poster T2-24

How green technology and nature-based interventions can influence human well-being

T Hitter (Buru)[1], E Kallay[2], M Cantor[1] and I Papuc[3]

[1] University of Agriculture Sciences and Veterinary Medicine, Faculty of Horticulture, 3-5 Calea Mănăştur, 400372, Cluj-Napoca, Romania;

[2] Babes Bolyai University, Department of Psychology, 1 Mihail Kogălniceanu, 400084, Cluj-Napoca, Romania

[3] University of Agriculture Sciences and Veterinary Medicine, Faculty of Veterinary Medicine, 3-5 Calea Mănăştur, 400372 Cluj-Napoca, Romania

E-mail: hittertimea@yahoo.com

Abstract. Technology in the future might rely on nature-based interventions, since it may improve the connection between people and greenspaces. In many modern societies, urbanization, resource exploitation, and lifestyle changes have diminished humans' possibilities to get in contact with nature. Considering the role of the natural environment, and the relationship between people and plants, additional principles of social and therapeutic horticulture can be explored, as meaningful activities, within a social environment or context. Less access to green spaces can affect people's life, reflected by a constantly increasing portion of the population which has presented significant symptoms of stress. Based on several completed questionnaires about therapeutic landscapes, this pilot study investigates the quantitative and qualitative aspects relevant for accessibility metrics and green spaces addressing these aspects in relation to people's well-being. Given the general evidence-based practice, nature-based interventions as therapeutic horticulture can reduce levels of the stress hormone (as cortisol), contribution of kynurenine as a biomarker, blood pressure, obesity, diabetes, ADHD symptoms and mental disorders by using structured natural green technologies as gardening programs in nature.

Poster T2-25

Design of novel antimicrobial peptides using a three-stage *in silico* approach

L Buimaga-Iarinca, A Farcas, C Floare and L Janosi

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: lorant.janosi@itim-cj.ro

Abstract. One of the main concerns in world public health is the increase in antimicrobial resistance. An important cause is bacteria developing resistance against naturally occurring antimicrobial peptides (AMPs), which are host defensive peptides with high selectivity of interaction with bacterial cells over mammalian cells. The *in silico* design strategy can be divided in three main stages. First, we used molecular docking simulations of specifically selected peptides from PepBank peptide database to bacterial and mammalian membrane models, in order to reduce the large amounts of available peptides. Second, we used molecular dynamics simulations to propose a list of potential candidates, whose affinities to bacterial and mammalian membrane models were calculated in the third stage. We found that combining these three methods is an efficient and relatively fast in silico approach that can be used to propose a reasonable number of potentially effective novel AMP candidates to be further tested and validated using experimental techniques. **Acknowledgements:** This work was supported by a grant of Ministery of Research and Innovation, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2016-0032 within PNCDI III.

Poster T2-26

Binding affinity of the intermolecular interaction between imatinib with α-1 glycoprotein

M Mic, A Pîrnău, C G Floare and M Bogdan

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: mihaela.mic@itim-cj.ro

Abstract. Imatinib is a selective tyrosine kinase inhibitor, successfully used for the treatment of chronic myelogenous leukaemia and gastrointestinal stromal tumors. Binding of drugs to proteins influence their pharmacokinetic and pharmacodynamics action. In the blood, the drug is distributed in the body in the free form or bound to plasma protein. Albumin and α-1 glycoprotein (AGP) are plasma proteins with the highest affinity for drug substances. Drugs which are weak acids mainly bind to plasma albumin, while drugs that are bases have affinity for α-1 glycoproteins. The main goal of this study is to quantitatively evaluate the interaction between imatinib and α-1 glycoprotein to characterize the nature and forces underlying the formation of a molecular complex. To fulfil this goal, we analyzed their interaction using ITC, NMR and molecular docking. **Acknowledgements.** This work was financially supported by Ministry of Research and Innovation, Romania, through the Core Program, Project PN 19 35 02 01.

Poster T2-27

Insights into selective incorporation of naturally-occurring flavonoids into metal-organic frameworks

M Miclăuș, A C Moț and I Grosu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: maria.miclaus@itim-cj.ro

Abstract. Seven flavonoids have been assessed in terms of their ability to incorporate into metal-organic frameworks: MIL-100 and MIL-101. The degree of uptake and release has been evaluated using UV-vis molecular absorption spectroscopy and high-performance liquid chromatography and appears to be strongly associated with their chemical structures. These findings leaded to experimental trials involving flavonoid separation from their mixtures and they proved to be successful. Flavonoid release from their MOF complexes has been optimized and kinetically-characterized using physiologically relevant conditions. Different behaviour for flavonoid release has been revealed and appears to be strongly dependent upon their iron-chelating power. Quercetin leads to unique chemical modifications which were further investigated using NMR and MS spectroscopies. Comparative analysis of the obtained flavonoid-MOF complexes has been performed by means of solid diffuse reflexive spectroscopy and X-ray diffraction on powder. Moreover, the antioxidant capacity of the flavonoid-MOF complexes has been tested using free radical scavenging assays, revealing their beneficial slow-acting property. **Acknowledgements**: Financial support from the Ministry of Research and Innovation—MCI, Core Programme, Project PN19 35 02 01.

Poster T2-28

Quality assessment of Valea Șesii stream near a cooper mine tailing pond

A Moldovan[1,2], M A Hoaghia[1], V Băbălău-Fuss[1,3], M Roman[1], M Tofană[3] and V Micle[2]

[1]INCDO-INOE2000, Research Institute for Analytical Instrumentation, ICIA Cluj-Napoca Subsidiary, 400293 Cluj-Napoca, Romania

[2]Technical University, Faculty of Materials and Environmental Engineering, 400641, Cluj-Napoca, Romania

[3]University of Agricultural Sciences and Veterinary Medicine Cluj-Napoca, 400372 Cluj-Napoca, Romania

E-mail: anamoldovan@icia.ro

Abstract. Roșia Poieni, a large copper mine from Arieș basin, produces tons of copper/year, the resulted sterile beingdeposited in Geamăna tailing pond located in the vicinity of Valea Șesii, one of the Arieș River tributaries, contributing decisively to the quality of its water. The study aims to assess the quality status of Valea Șesii using a complex green technology, combining chemical analysis and biomonitoring methods in order to establish the environmental trend of the catchment. A sampling campaign has been done along the stream, during the 2019 cold season. pH, EC, TDS, heavy metals (Cd, Pb, Cr, As), micro- (Zn, Mn, Cu, Ni, Co) and macronutrients (Mg, Ca, K, Na, S, N), BOD, chlorophyll a and b were analyzed in order to establish both the quality status of the surface water and the capacity of the existing microorganisms.The surface water quality is relatively good, with a circum-neutral 7.7 pH, 1436 µS/cm EC, TDS of 119 ppm, BOD of 4.2 mgO_2/L, but rather small values of nutrients. The presence of chlorophyll a and b was noticed (1.95 µg/mL and 4.76 µg/mL). A correlation between the nutrients content and the chlorophylls values was observed, while the chlorophylls values increases, the content of nutrients decreases.

Poster T2-29

^{1}H NMR relaxometry, FT-IR and Vis-near IR spectroscopy used for the characterization of personal care cosmetics

D Moldovan[1], R I Chelcea[1], A-M Biriș[1], D Șipoș[1] and R Fechete[1,2]

[1] Technical University of Cluj-Napoca, Faculty of Material and Environmental Engineering, 103-105Muncii, 400641, Cluj-Napoca, Romania

[2] Babeş-Bolyai University, Faculty of Physics, 1 Mihail Kogălniceanu, 400084, Cluj-Napoca, Romania

E-mail: rfechete@phys.utcluj.ro

Abstract. Personal care cosmetics have an important role in our social lives. Therefore, cosmetic science is a fast-moving area, with increasing constraints and limitations in the choice of cosmetic ingredients. Since personal care products are used in direct contact to human skin or hair. The use of expired cosmetics can lead to dramatic consequences for skin or hair health. ^{1}H NMR relaxometry, FT-IR and Vis-near IR spectroscopy were used to assess the effects of facial moisturizing creams on the natural skin, depilatory creams on wool, degradation factors on foundation creams and makeup products. The measured CPMG decays were analysed by inverse Laplace-like transform to obtain the distribution of transverse relaxation time T_2 associated with different ^{1}H pools. A large amount of hydration water was observed at smallest T_2-values. In FT-IR spectra important changes in the characteristic features are observed in the fingerprint region (wavenumber smaller than 1800 cm^{-1}). All cosmetic samples present a certain absorption in the ultraviolet region being also designated as sunscreen products. The anti-age cream and insulating skin cosmetics like foundation cream present a large absorption in the nearIR domain. Principal component analysis (PCA) was used for an advanced characterization of personal care cosmetics.

Poster T2-30

Theoretical DFT and experimental Raman spectroscopy study of cylindrospermopsin cyanotoxin

Cs. Müller Molnár[1,2], S Cintă Pînzaru[2], V Chiș[2], D A Magdas[1] and B Glamuzina[3]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Babeş–Bolyai University, Biomedical Physics, Theoretical and Molecular Spectroscopy Department, Kogălniceanu 1, 400084 Cluj Napoca, Romania

[3] University of Dubrovnik, Department for Aquaculture, Ćira Carića 4 20000 Dubrovnik, Croatia

E-mail: csilla.molnar@itim-cj.ro, simona.cinta@phys.ubbcluj.ro

Abstract. Cylindrospermopsin (CYN), a biotoxin originated from several cyanobacteria species is easily dissolved in environmental water columns when the responsible bacteria species blooming occurs. Such events may result in harmful outbreaks via human exposure to CYN through drinking water, recreational activities and by consuming foods in which the toxin may have bio-accumulated. Therefore, it is crucially important to acquire solid knowledge on their occurrence, molecular characterization, chemical behaviour in specific conditions, to be able to adopt adequate monitoring and surveillance program implementation. Current approaches on certain cyanobacteria raised difficulties in understanding and interpretation of the Raman signal from live cyanobacteria metabolites, therefore, we conducted a comprehensive theoretical DFT and experimental Raman approach to correctly assign the characteristic Raman modes of free CYN.

Poster T2-31

Chemometric analysis applied for the identification of DNAs from *Salmonella* serovars, before and after UV irradiation

C M Muntean[1], A Fălămaş[1], A M R Gherman[1], A Tăbăran[2] and R Ştefan[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]University of Agricultural Sciences and Veterinary Medicine, Faculty of Veterinary Medicine, 3-5 Calea Manastur Str., 400372 Cluj-Napoca, Romania

E-mail: cmuntean@itim-cj.ro

Abstract. Hierarchical Clustering Analysis (HCA) and Principal Component Analysis (PCA) were used to identify the similitudes between FT-IR DNAs spectra of inter- and intra- serovar groups, before and after UV irradiation. HCA, performed in Matlab R2016b, assigned spectra to clusters based on similarity. The first step consisted of calculating the distance between the spectra using the standardized Euclidean distance. The next step consisted of grouping the spectra into a hierarchical cluster tree by linking pairs of spectra that are in close proximity, based on the distances previously calculated. The final step is to obtain the dendrogram plot and cut the hierarchical tree into clusters. PCA is a multivariate analysis method, as well, suitable for pattern recognition. For further analysis we used the Unscrambler X 10.4. The first three principal components (PCs) brought the most contribution to the total variance and were plotted as three-dimensional PCA scores to observe the distribution of each DNA spectrum.
Acknowledgments: This work was supported by a grant of the Romanian Ministery of Research and Innovation, Core Programme, Project PN 19 35 02 01.

Poster T2-32

Nanoimmunosorbents based on functionalized SiO_2, Fe_2O_3 and Au nanoparticles used in homogenous nanoELISA technique

L Neagu[1], I Dorobanţu[1], C C Mustăciosu[1], R D Stoica[1], C Coman[2], D Ancuţa[2], R Turcu[3] and A Nan[3]

[1] Horia Hulubei National Institute for Physics and Nuclear Engineering (IFIN-HH), 30 Reactorului, Magurele, 077125 Bucuresti, Romania

[2] "Cantacuzino" National Institute of Medical-Military Research and Development, 103 Splaiul Independenței,050096 Bucuresti, Romania

[3] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: liviahar@nipne.ro

Abstract. Nanoimmunosorbents are functionalized nanoparticles with antibodies or antigens, which can be used in immunochemical dosing techniques. The paper presents the procedures for the obtainment of different types of nanoimmunosorbents based onSiO_2, Fe_2O_3 and Au used in homogenous nanoELISA technique for the detection of the pesticide 3,6-dichloro-2-methoxybenzoic acid (dicamba). Dicamba is used as broad-spectrum pesticide in agriculture and its remaining require high sensitivity analysis like ELISA in order to establish the contamination level of the alimentary products and the environmental factors. The immune reaction between the obtained nanoimmunosorbents and dicamba analyte, both in suspension, used in nanoELISA has the advantage of minimizing the diffusion distances between antigen and antibody and time to reach the chemical equilibrium in comparison with heterogeneous ELISA technique.

Poster T2-33

Chokeberry anthocyanins localization and visualization enhancement via Naturstoff reagent A in B16-F10 melanoma cell line

M Nistor[1], D Rugină[2], M Focșan[3], M Cenariu[2], A Pintea[2] and C Socaciu[1]

[1]University of Agricultural Sciences and Veterinary Medicine, Faculty of Food Science and Technology, 3-5 Calea Manastur, Cluj-Napoca, Romania
[2]University of Agricultural Sciences and Veterinary Medicine, Faculty of Veterinary Medicine, 3-5 Calea Manastur, Cluj-Napoca, Romania
[3]Babeș-Bolyai University, Faculty of Physics, 1 Mihail Kogalniceanu, Cluj-Napoca, Romania

E-mail: nistor.madalina@usamvcluj.ro

Abstract. Anthocyanins are bioactive compounds with protective properties against different types of cancer, including melanoma. Currently, there is no evidence to what extent anthocyanins are taken up by the melanoma cells. In this context, our aim was to determine cellular concentration and distribution of the anthocyanins in melanoma B16-F10 cells. Anthocyanins were extracted from chokeberries, purified through the SPE technique and quantified via HPLC/PDA analysis. Anthocyanins (92 µM Cyanidin-3-glucoside) proved to exert cytotoxicity on B16-F10 melanoma cells, according to WST-1 assay. Anthocyanins were taken up by melanoma cells, their cellular concentration being quantified by HPLC analysis. In order to easily follow their journey inside the B16-F10 cells, we bound them to a fluorescent compound like Naturstoff Reagent A (NSRA). It is known that anthocyanins express intrinsic fluorescence of rather low intensity.NSRA enhanced the fluorescence of the anthocyanins, with 86.2% of the cells expressing fluorescenceafter 2h, respectively with 61.5% after 24h as flow cytometry results prove. Therefore this enhanced fluorescence of anthocyanins enabled a better visualization of the anthocyanins inside the melanoma B16-F10 cells, sustaining NSRA to be a useful tool in studies required for distribution and visualization ofanthocyanins in melanoma cells.

Poster T2-34

Plastering Mortar with Organic Natural Polymers Studied By ^{1}H NMR relaxometry

A O Pintea[1], D L Manea[1], C Aciu[1], E Jumate[1] and R Fechete[2]

[1] Technical University of Cluj-Napoca, Faculty of Civil Engineering. 15C Daicoviciu, 400020 Cluj-Napoca, Romania

[2] Technical University of Cluj-Napoca, Department of Physics and Chemistry, 25 G. Baritiu, 400027 Cluj-Napoca, Romania

E-mail: alexandra.pintea@ccm.utcluj.ro

Abstract. Modern studies onconstruction buildings revealed the use of organic natural polymers as additives for the construction materials. It was demonstrated that by using these additives in composition of plastering mortars the mechanical properties and impermeability was improved. Ten recipes of plastering mortars, with and without organic natural polymers such as casein, rice and egg were studied by 1D ^{1}H NMR relaxometry. For the determination of the T_2 transverse relaxation time distributions, the acquired CPMG decays were analysed using a fast Laplace inversion algorithm. These distributions were obtained for wet and dry plaster mortars which were measured after 28 days from preparation during the hydration of mineralogical components. In almost all cases, the distributions of transverse relaxation times T_2 were characterized by four components associated with hydration water and water inthree types of pores of different dimension. The relaxation ratio ($1/T_2$) of hydration water were correlated with mechanical resistance at elongation and compression and water absorption degree. Among replacement additives the plaster mortar with casein increases the mechanical properties and the formula with egg reduce the water permeability.

Poster T2-35

The statistical determination of the similarity of the organic composition of some Black Sea sediments by nuclear magnetic resonance (NMR)

A Pîrnău, C G Floare, I Feher, M Mic, R H Puşcaş, I Turcu and A Măgdaş

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: adrian.pirnau@itim-cj.ro

Abstract. Nuclear magnetic resonance (NMR) spectroscopy will be used for statistical determination of the similarity of the organic composition of soil samples extracted from the bottom of the sea, drilled at different depths and locations. Preliminarily, a sample preparation method has been implemented. On the following the acquisition and processing of the spectra was performed using TopSpin 2.1 software, whenwe corrected the phase of the signal and we calibrated the spectra relativelyto a reference signal - tetramethylsilane (TMS). The measured spectra are then compared by statistical methods using linear discriminant analysis (LDA).The LDA analysis was separately applied on four spectral ranges: Area 1 (9–6 ppm), Area 2 (4.7–3.45 ppm), Area 3 (3–1.66 ppm) and Area 4 (1.66–0.5 ppm), on 21 samples collected from different places and at different depths. **Acknowledgements.** This work was supported by a grant of the Romanian Ministery of Research and Innovation, CCCDI – UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0178/ 24PCCDI/2018, within PNCDI III.

Poster T2-36

A simple method for obtaining high purity phycobiliproteins

A S Porav[1,2], M Bocaneala, A Falamas[2], L Barbu[1,2] and N Dragos[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Babeş-Bolyai University, Faculty of Biology and Geology, 3-5 Clinicilor Street, 400006, Cluj-Napoca, Romania

E-mail: sebastian.porav@itim-cj.ro

Abstract. Phycobiliproteins are a class of globular, water soluble proteins, mostly encountered in cyanobacteria and red algae, where they assemble in the photosynthetic light harvesting antenna called phycobilisome. Phycobiliproteins can be classified based on their spectroscopic properties in phycocyanin, allophycocyanin, phycoerythrin and phycoerythrocyanin. Due to their properties like high water solubility, non-toxic corlorant, bright fluorescence, large Stokes shift and many conjugation sites, this class of proteins have a broad range of applications in biotechnology, cosmetics, immunological assays, pharmaceutical and nutraceuticals industries. Due to the increasing demand for these proteins, improving the extraction and purification process in a cost-efficient manner is essential. Here we report an optimized two step method for obtaining pure phycobiliproteins with high yield. This method involves the use of an aqueous two-phase system (ATPS) based on PEG and different phosphate salts for initial fractionation of the soluble proteins followed by size exclusion chromatography. To test and optimize the method we used several species of cyanobacteria with different phycobiliprotein composition. In all cases we obtained the different phycobiliprotein (phycocyanin, allophycocyanine and phycoerythrin) at a reagent grade purity (>3.5) based on the ratio between their specific absorbencies and absorbance at 280 nm. This work was supported by a grant of the CCCDI-UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0010 and the Core Program, Project PN 19 35 02 01.

Poster T2-37

Development of tomato (*Solanum lycopersicum L.*) seedlings under the action of extremely low frequency magnetic field in a controlled environment condition

M Răcuciu

Environmental Sciences and Physics Department, Faculty of Sciences, Lucian Blaga University of Sibiu, 5-7 Dr. I. Ratiu, 550012 Sibiu, Romania

E-mail: mihaela.racuciu@ulbsibiu.ro

Abstract. In order to evaluate the effects of extremely low frequency magnetic field on growth of tomato seedlings (*Solanum lycopersicumL.*), an environmental controlled experiment was conducted during 2016-2017. After three weeks of germination of seeds and ulterior growth, each tomato seedling was transferred on soil in separate recipient and irrigated with 5ml distilled water daily. After, each seedling had been exposed one by one to extremely low frequency (50Hz) magnetic field with different values of magnetic flux density (1-2-3 mT) and for different durations of daily exposure. For both type of samples, control and exposed plants, were determined the effects of magnetic field on assimilatory pigments level at different step of growth under daily magnetically exposure. Results indicated that the exposure to magnetic field increased the chlorophylls level for lower magnetic flux density and lower exposure duration, respectively. The humidity of the fresh tissue was affected by the magnetic field presence during the fifty days of growth.

Poster T2-38

Generation of Reactive oxygen species (ROS) in hepatocarcinoma cells after proton irradiation

M Răileanu, M Straticiuc, R Andrei, D Iancu, M Radu and M Bacalum

"Horia Hulubei" National Institute of Physics and Nuclear Engineering, Măgurele, Romania

E-mail: mina.raileanu@nipne.ro

Abstract. In order to assess the effects induced by proton radiation into hepatocarcinoma cells, we used IFIN-HH existing facility - a 3 MV TandetronTM accelerator. The proton beam was extracted into air through a 1 μm thick Si_3N_4 window and the irradiations were performed at 3 cm distance from the window. The chamber in which the cells were grown for irradiation was specially designed for the experimental set-up. In vitro studies were performed on HepG2 human hepatocarcinoma cells, irradiated at different doses between 0.5 - 3 Gy. Cell viability and colony formation were used to assess the influence of radiation on cell replication. We also checked how the cell cycle is affected by proton irradiation. Finally, the intracellular generation of reactive oxygen species was measured at different times after irradiation. The results obtained show a dose dependent effect for ROS formation and cell cycle arrest.

Poster T2-39

Hazardous pollutants generated by 1997-1998 generation of printed circuit boards

D Simedru, A Moldovan, V Babalau-Fuss, A Hoaghia, O Cadar, A Torok, E Levei, M Kovacs and O Todor-Boer

INCDO-INOE 2000, Subsidiary Research Institute for Analytical Instrumentation Cluj-Napoca, 67 Donat, 400293Cluj-Napoca, Romania

E-mail: dorina.simedru@icia.ro

Abstract. Due to the high quantity of printed circuit boards waste generated in the last years, it is imperative to quantify their environmental impact and to find recycling solutions. In order to quantify the environmental impact of 1997-1998 generation of printed circuit boards, a migration test was performed. The following parameters were determined: metals, fluoride, chloride, sulfates, phenol index, dissolved organic carbon, total organic carbon, total dissolved substance, BTEXs, PCBs and petroleum products. The analyses were performed using sensitive, high performance analytical techniques. The results were compared with those stipulated in the legislation in force in order to identify the appropriate waste category for their storage. The values obtained for Cu, Ni, Pb, Sb and Zn are higher than the maximum admitted levels for their acceptance in inert waste deposits. While the values of Cu and Zn are decreasing from 51.6 to 4.03 mg/kg for Cu and from 23.6 to 8.79 mg/kg for Zn, the values of Ni and Pb are increasing from 0.75 to 1.55 mg/kg for Ni and from 8.72 to 34.0 mg/kg for Pb from 1997 to 1998. These results show that finding a solution for therecycling 1997-1998 generation of printed circuit boards is being mandatory.

Poster T2-40

Immunochemical characterization of anti dicamba antibodies

R D Stoica[1,2,3], L Neagu[1], I Dorobanţu[1], C C Mustãciosu[1], C Coman[4] and D Ancuţa[4]

[1] Horia Hulubei National Institute for Physics and Nuclear Engineering (IFIN-HH), 30 Reactorului, Magurele,077125 Bucuresti, Romania

[2] Faculty of Chemistry, University of Bucharest, 4-12 Regina Elisabeta,030018 Bucuresti, Romania

[3]University POLITEHNICA of Bucharest, 1-7 Gheorghe Polizu, 011061 Bucuresti, Romania

[4] "Cantacuzino" National Institute of Medical-Military Research and Development, 103 Splaiul Independenței, 050096 Bucuresti, Romania

E-mail: raluca.stoica@nipne.ro

Abstract. For the development of homogenous nanoELISA technique for detection of the residual pesticide 3,6-dichloro-2-methoxybenzoic acid (dicamba) is necessary to obtain polyclonal antibodies against dicamba. The immunization experiments were undertaken under national and international regulations concerning animal testing, with dicamba-bovine serum albumin as immunogenic conjugate, using a protocol approved by the ethics committee of "Cantacuzino" institute and authorized by DSVSA Bucharest. The gamma globulins are separated by the chemical method using $(NH_4)_2SO_4$ due to its higher efficiency. The selection of antisera is made according to their titre and affinity for the antigen. The obtained antibodies are tested by ELISA technique using as enzymatic marker dicamba-alkaline phosphatase and are also presented evaluating procedures of the equilibrium constant (affinity constant), forming and dissociation rate constants of the immune complex as well as the avidity (Gibbs free energy). The anti dicamba antibodies obtained in this study presents different affinities and all of them recognize the antigen.

Poster T2-41

Molecular docking and experimental evidences for the allicin immunostimulatory mechanism

V Toma[1,2], A Farcaș[1,2], R Gherman[1], A B Țigu[3], E Fischer-Fodor[3,4], B Sevastre[5], I Roman[6] and M Pârvu[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Babeș-Bolyai University, Department of Molecular Biology and Biotechnologies, 1 Kogălniceanu, 400015, Cluj-Napoca, România

[3] Research Centre for Advanced Medicine ``Medfuture``, University of Medicine and Pharmacy ``Iuliu Haţieganu`` 400349 Cluj-Napoca, Romania

[4] Institute of Oncology ``Ion Chiricuță``, Cluj-Napoca, 42 Republicii Street, Cluj-Napoca, 400015, Romania

[5] Department of Pathophysiology, University of Agricultural Sciences and Veterinary Medicine, Cluj-Napoca, 400372, Romania

[6]Institute of Biological Research Cluj-Napoca 400113, branch of NIRDBS București, Romania

E-mail: vlad.al.toma@gmail.com

Abstract. We purposed that S-allyl-mercaptogluthatione (SAMG) molecule plays an agonistic function like polyanionic molecules, modified LDL or polysachharides on scavenger receptors class A (SRs-A) Colec12 from macrophages and generate *via* B cells stimulation a nonspecific humoral immune response marked by immunoglobulin increasing concentration whereas white blood cells number is not changed. Also, we investigated the B cells could express scavenger receptors which allow the direct stimulation by SAMG and finally determined immunoglobulin increasing concentration. Therefore, the purpose of the current study was to investigate the mechanism responsible for the allicin immunostimulation.

Poster T2-42

Crystal structure of 2α,17α-Dimethyl-4,5α-dihydrotestosterone

A Turza[1], G Borodi[1], S Albert[1] and P A Camarasan[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]Faculty of Environmental Science and Engineering, Babes-Bolyai University, 30 Fantanele, 400000 Cluj-Napoca, Romania

E-mail: aturza@itim-cj.ro

Abstract. The crystal structure of 2α,17α-Dimethyl-4,5α-dihydrotestosterone has been determined by X-ray single crystal diffraction. The drug belongs to anabolic-androgenic steroids class and was found to crystallize in $P2_12_12_1$ space group of the orthorombic crystal system with the following unit cell parameters: a=11.3132(3) Å, b= 13.2281(3) Å, c=12.3303(3) Å, $\alpha=\beta=\gamma=90^0$. The A, B and C rings from the steroid skeleton depicts chair conformations, while ring D exists as 13β distorted envelope conformation. The supramolecular self-assembly is aggregated by O-H...O hydrogen bonds. Hirshfeld surface analysis shows that the H...H intermolecular interactions dominates the structure and the H...O/O...H interactions to a lesser degree.

Poster T2-43

Conformational study of Febuxostat molecule correlated to its co-crystallization ability with carboxylic acids

D Ungur[1], M Prața[1], D Coman[1], C Brăilă[1], AMR Gherman[2], I Kasco[2], X Filip[2] and M Pop[1]

[1] TeraCrystal, 400293 Cluj-Napoca, Romania

[2] Molecular and Biomolecular Physics Department, National Institute for R&D of Isotopic and Molecular Technologies, 400293 Cluj-Napoca, Romania

E-mail: doriana.ungur@teracrystal.com

Abstract. Febuxostat (FB), a non-purine selective inhibitor of xanthine oxidase used for lowering the serum uric acid levels, possesses a low aqueous solubility, which is characteristic to class II of drugs according to the Biopharmaceutics Classification System (BCS). With the aim of improving the aqueous solubility of FB we investigated its ability to form co-crystals by applying modeling techniques followed by co-crystallization experiments. Conformation of the febuxostat molecule was studied by molecular mechanics calculations using systematic searching as well as two stochastic methods: random sampling and Boltzmann jump. Aclustering methodology developed to analyze molecular similarity revealed the unique conformers of FB. Furthermore, the energy window of the conformers that could be obtained by co-crystallization was derived from comparison with the FB crystal structures reported in Cambridge Structural Database (CSD). Finally, co-crystal experimentation resulted in the identification of six novel co-crystals with carboxylic acids. Our work indicates that conformational search is a promising technique for guiding the co-crystallization ability of drug molecules. **Acknowledgement** The authors acknowledge financial support from the Ministry of Research and Innovation - MCI, Operational Program Competitiveness, POC Project 18/01.09.16, SMIS Code 105533.

Section T3:

Energy Efficiency and High-Tech Engineering

Oral T3-1

FPGA Technology in High Energy Physics

B Belean on behalf of ITIM ATLAS Group

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: bogdan.belean@itim-cj.ro

Abstract. New generation hadron colliders aim to achieve an instantaneous luminosity corresponding to 200 simultaneous proton-proton interactions per bunch crossing. Moreover, in terms of collisions frequency, a bunch spacing with the order of magnitude of a few tens of ns is expected. In order to readout and store all the events for each bunch crossing, powerful acquisition system and computing architectures are needed to build particle detectors. The main benefits of using FPGA technology in developing digital system for the detectors readout and trigger processes are presented. **Acknowledgments.** This paper was financially supported from the MCT, Nucleu-Program, project nr.PN 19350101 and PNCDI III, CERN/08 ATLAS -ATLAS Experiment at the LHC

Oral T3-2

Innovative Mechanics for Particle Detectors

G Popeneciu on behalf of ITIM ATLAS Group

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: gabriel.popeneciu@itim-cj.ro

Abstract. To advance on the territory of high energy physics new detectors with higher sensibility and reliability are required. To face up the challenges of the future High Luminosity - Large Hadron Collider (HL-LHC) at CERN Geneva, designed to achieve unprecedented collision energy and luminosity, is proposed an upgrade of the Tile Calorimeter detector, one of the detectors of the ATLAS experiment. Innovative mechanical solutions were developed to implement the “mini-drawer” concept for the new Tile Calorimeter read-out electronics. The benefits of the new mechanics are a better accessibility to the electronics for maintenance, higher reliability and radiation resistance. **Acknowledgments.** This paper was financially supported from the MCT, Nucleu-Program, project nr.PN 19350101 and PNCDI III, CERN/08 ATLAS -ATLAS Experiment at the LHC

Oral T3-3

Concentrated solar power and Stirling engine

V Rednic, A Bot, E Bruj, R Gutt, S Gergely, R Pop, R Gavrea, S Pogacian, D Zotoiu and N Aldea

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: vasile.rednic@itim-cj.ro

Abstract. Solar concentrators with Stirling engine are environment friendly systems that produce electricity from renewable clean energy. In this contribution a hybrid system, comprising of a number of solar concentrators, heat receivers and a Stirling engine coupled to an electric generator is presented. The system includes a combustion chamber to compensate for reduced/absent sunlight, so that a constant temperature of thehot side of the Stirling engine is maintained, irrespective of the sun conditions. The system is mounted on a two-axis solar tracking system. The thermal energy generated by the concentrated solar energy is transferred from the thermal receiver by the gaseous thermal agent directly into the Stirling engine combustion chamber. The Stirling engine exhaust contains two heat recovery units in order to increase the total system efficiency. The thermal agent is preheated in the first heat recovery unit before it reaches the thermal receivers located in the focal point of solar concentrator, whilethe second heat recovery unit includes cooled thermoelectric elements to convert the wasted thermal energy into electricity. Their cooling system is connected to that of the Stirling engine and includes a heat exchanger for recovering heat in the form of hot water. **Acknowledgment.** This paper was financially supported from the MCI, Nucleu-Program, project nr.PN 19 35 01 01.

Oral T3-4

Techno-Economic Analysis and Comparison of the new Gas Switching Combustion Technology

S Szima[1], C Arnaiz del Pozo[2], S Cloete[3], Á Jiménez Álvaro[2], A M Cormoș[1], S Amini[3] and C C Cormoș[1]

[1] Babes - Bolyai University, Cluj-Napoca, Romania

[2] Universidad de Politecnica de Madrid, Madrid, Spain

[3] SINTEF Industry, Trondheim, Norway

E-mail: szima@chem.ubbcluj.ro

Abstract. Gas switching combustion (GSC) is a modified form of chemical looping combustion. The same GSC reactor containing oxygen carrieris used for the oxidation and reduction stages to avoid solid circulation. This being the main advantage of the technology. The plant layout was selected based on previously reported data incorporating the GSC technology. The proposed power plant in this work has a net power output of 368 MW with the efficiency being over 40 %, similar to the efficiency of an IGCC power plant without CCS. The specific CO_2 emission of the plant is below 65 kg/MWh, with a CO_2 capture rate over 90 %. The capital cost of the GSC reactor was obtained using both experimental and simulation results with a close attention on the high temperature and pressure. For the rest of the system cost correlations were used. The levelized cost of electricity is in the range of 85 €/MWh and it was calculated assuming a net present value of 0 at the end of the economic lifetime. The proposed GSC power plant shows great promises both from technical and economic point of view performing significantly better than conventional gasification power plants with CO_2 capture.

Oral T3-5

Temperature variation inside Data Center by airflow control - 3D model and simulation

M R C Trușcă[1], J Nagy[1], S Albert[1] and F Fărcaș[1] and S Brad[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Technical University of Cluj-Napoca, 28 Memorandumului, 400114-Cluj-Napoca, Romania

E-mail: radu.trusca@itim-cj.ro

Abstract. Cooling is a major cost factor in Data Centers, if it is implemented improperly, the power required to cool the Data Center can reach or exceed the power used to run the IT equipmentsthemselves. Cooling is also often the limiting factor in Data Center capacity (heat removal may be a bigger problem than obtaining the energy needed for computing equipment).In order to optimize the temperature in INCDTIM Data Center, more stages were taking into account as follows: (i) collecting input data and realizing the 3D model of the current situation; (ii) designing different solutions for directing the airflow in the Data Center; (iii) implementation of the cooling solution found; (iv) tracking system operation and adjusting parameters according to the obtained values. The aim of this work was to simulate the variation of the temperature by air flow control. The 3D model of the Data Center was created in CAD Software and the simulation of the air flow was done in Ansys CFD. **Acknowledgement:** This work was carried out in the framework of Romanian-JINR cooperation (Order 396-73/27.05.2019 and Order 397-75/27.05.2019).

Oral T3-6

New plasma applicator design for the improved activation of large surfaces

C D Tudoran[1,2] and M Coroș[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] **CETATEA**, Center for Research and Advanced Technologies for Alternative Energies

E-mail: ctudoran@itim-cj.ro

Abstract. We present a patent pending cold plasma applicator, designed and built specifically for the plasma treatment of large surfaces of materials. The plasma applicator was used in our laboratory for the activation of textile and leather fabric surfaces with the aim to improve their hydrophilic and hydrophobic properties respectively. The plasma applicator generates an atmospheric pressure cold plasma discharge in a flowing gas (Ar, He, N_2, air, etc.) with a kinetic temperature of 36...40 ^oC, being suited also for the activation of temperature sensitive materials. Our plasma applicator design has two main advantages over the existing commercial systems (corona treaters and plasma jets): it allows the focused use of specific gases or gas mixtures for the treatment of slow responsive materials and it can also treat large surfaces of materials (widths in the order of thousands of milimeters) in a single pass.

Poster T3-1

Stirling engine's combustion chamber optimization

E Bruj, A Bot, V Rednic, S Pogăcean, Ș Gergely, R Pop, R Gutt and D Zotoiu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: emil.bruj@itim-cj.ro

Abstract. Due to the rising interest in the optimisation of the Stirling engine, this work considers a simulated design of a Stirling engine combustion chamber and discusses the thermal parameters, such as the heater temperature, the energy loss of the burning cavity, the temperature distribution inside the chamber as well as the ejected stream heat. The numerical results are performed in ANSYS Fluent, in order to obtain the temperature distribution, the velocity profiles and the heat flux. The initial setup is based on an existing combustion chamber for a Stirling engine, such that the numerical results are compared to experimental measurements. Based on this model, different structures for the combustion chamber are considered in order to increase the burning process efficiency. **Acknowledgment.** This paper was financially supported by MCI, Nucleu-Program, project no.: PN 19 35 01 01.

Poster T3-2

Automated photographic device for real-time monitoring of *in vitro* biological samples

A Ciorîță[1,2], V Surducan[1] and E Surducan[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]Babeș-Bolyai University, Faculty of Biology and Geology, 5-7 Clinicilor, 400006, Cluj-Napoca, Romania

E-mail: alexandra.ciorita@itim-cj.ro

Abstract. In microbiology it is crucial to closely supervise the development of microorganisms, and there are many external factors that may influence the outcomes. Our device helps eliminating some of those factors by reducing the human interaction with the biological samples to a minimal, continuous and long-term monitoring of the evolution of biological samples, and last but not least, eliminates the condensation that appears in time. The device has two replicas, each with: a digital camera mounted on a stand with an optical mirror positioned at 45°, a Petri dish situated above the digital camera, with biological sample and humidity absorbent system, and a LED lamp, transparent for electromagnetic field, with diffusion system, above the Petri dish. This device allows the observation of both electromagnetically stimulated and non-stimulated biological samples at the same time, making it possible to compare the results faster and in a less prone to error manner. Another advantage consists in the fact that a large variety of biological samples can be examined using this device, from bacteria, fungi, or algae, to *in vitro* plant crops, that may interact on a daily basis with environmental electromagnetic filed radiation. **Acknowledgments.** This paper was financially supported from the MCT, Nucleu-Program, project nr.PN 19350101.

Poster T3-3

An electric vehicle charging station powered by wind turbine

R A Felseghi[1], I Aşchilean[2], M S Raboaca[3], A Corbu[3] and C Filote[1]

[1] Faculty of Electrical Engineering and Computer Science, "Ştefan cel Mare" University of Suceava, Universităţii street, no.13, 720229 Suceava, Romania;

[2] Faculty of Civil Engineering, Technical University of Cluj-Napoca, Constantin Daicoviciu street no. 15, 400020 Cluj-Napoca, Romania;

[3] National Research and Development Institute for Cryogenic and Isotopic Technologies-ICSI, Uzinei Street, No. 4, P.O. Box 7 Raureni,240050 Ramnicu Valcea, Romania.

E-mail: andreea.felseghi@gmail.co

Abstract. Worldwide, political framework reaffirmed sustainable development as a central element of the international agenda and give a new impetus to the practical application of the global measures to combat the negative effects of human actions and for the environmental protection.The development of electric vehicles(EV) technology as a standard of energy efficiency in the transport sector has made important contributions in terms of reducing greenhouse gas emissions, but the success of implementing this concept directly depends on the alternatives for the use of clean energies through the various power generation systems that will be adopted.In this respect, the present work proposes a simultaneous approach to the two concepts with a particular role in the sustainable development of transport infrastructure, namely electric vehicles and alternative energies.This paper examines the possibility of charging EV batteries with clean energy using wind resources. An isolated system was designed, dimensioned and simulated in operation for an EV charging station with wind turbine and batteries as main components. The results were related to the energy, environmental and economic performance achieved.

Poster T3-4

Investigations on compensated ferrimagnetism in $Mn_2Co_{0.5}V_{0.5}Al$ Heusler alloy

R Gavrea[1,2], D Benea[2], R Hirian[2], O Isnard[3,4] and V Pop[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Faculty of Physics, Babeş-BolyaiUniversityCluj-Napoca, Kogălniceanu str 1,400084 Cluj-Napoca, Romania

[3] Université Grenoble Alpes, Institut Néel, Grenoble, F-38042, France

[4] CNRS, Institut Néel, 25 rue des Martyrs, BP 166x, F-38042 Grenoble cedex 9, France

E-mail: radu.gavrea@itim-cj.ro

Abstract. We present theoretical and experimental investigations on the electronic and magnetic properties of the $Mn_{2+\delta}Co_{1-\delta}V_{0.5}Al$ ($\delta = 0 \div 0.08$) and $Mn_{2+z}Co_{0.5}V_{0.5-z}Al$ ($z = -0.14 \div 0.08$) Heusler alloys. The electronic band structure calculations performed using the Korringa-Kohn-Rostoker (KKR) Green's function method show the dependence of the total spin moment on the preferential site occupation for different crystal sites and predict compensated ferrimagnetic behaviour for the compounds derived from $Mn_2Co_{0.5}V_{0.5}Al$ by slight variation on composition. Experimentally, $Mn_2Co_{0.5}V_{0.5}Al$ alloy is characterized by a nearly compensated ferrimagnetic behaviour with a low spontaneous magnetization of 0.29 μ_B/f.u. Further experimental investigations by tuning the Mn content in $Mn_2Co_{0.5}V_{0.5}Al$ alloys have been performed in order to achieve the fully compensated ferrimagnetic behaviour which is of particular importance for spintronics. **Acknowledgments.** This paper was financially supported partially from the MCT, Nucleu-Program, project nr. PN 19350101.

Poster T3-5

Development and Application of Confocal XANES System

G Chen[1,2], PAn[2], L Zheng[2], SChu[2], Y Du [3] and J Zhang[2]

[1] University of Chinese Academy of Sciences, Beijing 100049, China

[2] Beijing Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China

[3] Institute of Chemical and Engineering Sciences, Agency for Science, Technology and Research, 1 Pesek Road, Jurong Island 627833, Singapore

E-mail: chenguang@ihep.ac.cn

Abstract. As a powerful tool for determination of element distribution and chemical species with non-destructive investigated capacity, confocal XANES is widely used in archaeology, environmental science and chemistry. However, the adjustment of confocal is operated manually, which is time-consuming. We developed an alignment procedure based on evolutionary algorithm adjusting the confocal system, and the procedure was able to complete the adjustment process within 30 minutes. Sacrificial red glaze was investigated by the system. The glaze reveals a distinct layered structure. The ratio of Cu^0 to Cu^{1+} is positive correlated with the depth. Therefore, we propose an explanation of the mechanism of sacrificial red glaze's coloration, which proves to be promising for a non-destructive archaeology study.

Poster T3-6

Thermal receptor for capturing and converting concentrated solar energy

R Gutt, V Rednic, **E Bruj and A Bot**

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: robert.gutt@itim-cj.ro

Abstract. Solar energy, one of the most important renewable energy sources, can be used as a heat source for a Stirling engine. In this presentation, we investigate through numerical simulations and experimental measurements, different models of thermal receptors that capture and convert solar energy. The experimental assembly uses Fresnel lenses as solar concentrators in the focus of which are located the 3 different models of thermal receptor mounted on a two-axis solar tracking system. The numerical simulation used in this study is performed in ANSYS software, using the Fluent package to simulate working fluid flow. The simulation software enables the computation of temperature distributions, energy losses as well as energy transferred through the thermal receiver. The outlet temperature of the working gas is measured and comparted to the numerical ones for different inlet densities. **Acknowledgment.**This paper was financially supported from the MCI, Nucleu-Program, project no PN 19 35 01 01.

Poster T3-7

Green methods for the extraction of carbohydrate compounds from vine shoot waste

E Kovacs[1,2], D A Scurtu[1], L Senila[1], C Oana[1] , D E Dumitras[2] and C Roman[1]

[1] INCDO-INOE 2000, Research Institute for Analytical Instrumentation, 67 Donath, 400293 Cluj-Napoca, Romania

[2] University of Agricultural Sciences and Veterinary Medicine, 3-5 Manastur, 400372, Cluj-Napoca, Romania

E-mail: lacri.senila@icia.ro

Abstract. Annually large amounts of vineyard waste are produced from vine pruning. Romania has a vineyard of 183 thousand ha and produces 6.0 million hl of wine/annum, being ranked 10th in the world and 5th in Europe, after Spain, France, Italy and Portugal. Currently, waste is incorporated into the soil or burned in open field, leading to increased greenhouse gas emissions. The extraction of cellulose, hemicellulose and lignin from vine shoot waste is a primordial step for the integral valorization of these resources. The study aims to obtain carbohydrates from vine shoot waste from Romanian grape varieties by using an innovative method for the transformation of vine shoot waste into valuable compounds. Microwave pretreatments were performed using different operational conditions: temperature (150-180°C), residence time (10-30 min). The pretreated vine shoot waste was delignified with sodium chlorite for lignin removal and then enzymatically hydrolyzed using new types of enzymes (cellulase from Trichoderma reesei and β-glucosidase). A total of 40 g carbohydrates can be obtained from 100 g vine shoot waste. It can be concluded that the vine shoot waste could be used as raw material for bioethanol production by using a green technology in the context of circular economy objectives.

Poster T3-8

The bioenergy sector efficiency in the global demand context

E Kovacs[1,2], L Senila[1], D A Scurtu[1], C Roman[1] and D E Dumitras[2]

[1]INCDO-INOE 2000, Research Institute for Analytical Instrumentation, 67 Donath, 400293 Cluj-Napoca, Romania

[2]University of Agricultural Sciences and Veterinary Medicine, 3-5 Manastur, 400372, Cluj-Napoca, Romania

E-mail: eniko.kovacs@icia.ro

Abstract. In the context of the fossil fuels depletion, the bioenergy transition target objectives set by policy makers are increasingly challenging. There are massive negative ecological impacts in terms of deforestations, land use, emissions and GHG footprint, but also undesirable economic impacts. Science is struggling with the efficiency of the bio-chemical and thermodynamic processes; technology cannot achieve an entirely clean production at the expected performances and simultaneously curbdown the costs. The paper aims to perform a brief screening of the scientific, technical, social and economic basis for such a systemic orientation. The first section identifies the criteria and analyses the methodologies on which the major policies rely, the second section collects the experience feedback from science and industry and the third section reviews the past, current and future trends in comparison with the policy targets and delivers interpretations. By summarizing the bioenergy sector's efficiency, the paper tries to qualify the extent to which biomass can be a solution to the global energy demand.

Poster T3-9

Optimizing High-Harmonic Flux Using Artificial Neural Networks

K Kovács[1], A M M Gherman[1], M V Cristea[2] and V Tosa[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Chemical Engineering Department, Babeș-Bolyai University, Arany János 11, 400028 Cluj-Napoca, Romania

E-mail: kkovacs@itim-cj.ro

Abstract. We present a method based on artificial neural networks (ANN) - as an efficient mathematical modeling procedure - aimed to predict the outcome of high-order harmonic generation (HHG) experiments with previously unexplored parameters. The main goal is to provide quick help for attosecond science laboratories in designing experiments, such as ELI research centers. In this particular work we present the results obtained with an artificial neural network which we trained to predict the expected output of high-order harmonic generation process, while exploring a multi-dimensional parameter space. We argue on the utility and efficiency of the ANN model and demonstrate its ability to predict the outcome of HHG simulations. In this case study we present the results for a loose focusing HHG beamline, where the changing parameters are: the laser pulse energy, gas pressure, gas cell position relative to focus and medium length. The physical quantity which we predict here using ANN is directly related to the total harmonic yield in a specified spectral domain (20–40 eV). We discuss the versatility and adaptability of the presented method. Financial support is acknowledged to Core Program No. PN 19 35 02 01.

Poster T3-10

Assembly tools for the new Tile Calorimeter electronics

I Nadas on behalf of ITIM ATLAS Group

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: iuliu.nadas@itim-cj.ro

Abstract. The ATLAS experiment at LHC CERN Geneva will follow a new stage of development to face the challenges of the High Luminosity - LHC project. For the Tile Calorimeter, one of the ATLAS detectors, the current read-out electronics will be totally replaced. The new Tile Calorimeter electronics will be installed in 256 super-drawers that are based on mini-drawer concept. To reach the goal to assemble 2 super-drawers per day a dedicated assembly tools have to be designed and fabricated. To meets functional and technical requirements necessary in the assembly process and to confer to the user good manoeuvrability during the installation process, two different prototypes are designed and fabricated with the purpose to have the best solution ready to be produced. **Acknowledgments.** This paper was financially supported from the MCT, Nucleu-Program, project nr. PN19350101 and PNCDI III, CERN/08 ATLAS -ATLAS Experiment at the LHC

Poster T3-11

OPAL RT Technology: Proton-Exchange Membrane Fuel Cells

M S Raboaca[1,2,3,] **A Nasture**[1]**, A Corbu**[1]**and L Patularu**[1]

[1]National Research and Development Institute for Cryogenic and Isotopic Technologies-ICSI, Uzinei Street, No. 4, P.O. Box 7 Raureni, 240050 Rm. Valcea, Romania.
[2]Faculty of Electrical Engineering and Computer Science, "Ştefan cel Mare" University of Suceava, Universităţii street, no.13, 720229 Suceava, Romania;
[3]Technical University of Cluj-Napoca, Memorandumului Street, No. 28, 400114 Cluj-Napoca, Romania
[4]Computers and Automation Department, Universitatea Politehnica Bucuresti, Romania
ical University of Cluj-Napoca, Memorandumului Street, no. 28, 400114, Cluj-Napoca, Romania.

E-mail: simona.raboaca@icsi.ro; ana.nasture@icsi.ro

Abstract. The goal of this paper is to simulate in real-time a proton exchange membrane fuel cell (PEMFC). This paper presents different types of fuel cells, a mathematical model for PEMFC, OPAL RT technology, real-time simulation architecture, conditions for the Simulink / MATLAB mathematical model implementation on the RT-LAB platform using the OPAL-RT simulator. The real-time simulations represent a great advantage in research / design by corroborating three crucial factors: rapidity of implementation, flexibility in development, predictability of results. In this paper was presented the simulation system OPAL-RT as an alternative in research / development of PEM fuel cells. The most important advantage of this simulator is the connectivity between RT-LAB and Simulink. OPAL-RT is using advantages of HIL (hardware-in-the-loop) and SIL (software-in-the-loop) PIL (power-in-the-loop) for innovating, designing, testing and analysing power electronics systems and power systems.

Poster T3-12

Tightness check of leakless water cooling systems

S Pogacian on behalf of the ATLAS group

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: sergiu.pogacian@itim-cj.ro

Abstract. Leakless Cooling Systems (LCS) are specially designed to avoid dangerous leakage of liquid. The LCS is used for applications where leakage would have fatal consequences, like in the case where sensible electronic components have to be cooled. In principle the LCS is a closed system working with sub-atmospheric pressures. Since the pressure in the cooling pipes is lower than the atmospheric pressure a leak in the circuit does not result in leakage of cooling liquid but air will be sucked in. This additionally allows to detect leaks in the system because it implicates an increase in pressure which can be monitored. This paper is aimed to present the working principle of a water LCS and a method to check tightness of cooling circuit before commissioning. The cooling system of the Tile Calorimeter, one of the detectors of the ATLAS experiment at LHC-CERN, is presented as study case. **Acknowledgments.** This paper was financially supported from the MCT, Nucleu-Program, project nr.PN 19350101 and PNCDI III, CERN/08 ATLAS -ATLAS Experiment at the LHC

Poster T3-13

Study of optimization for different micro-hydro power plant construction, in order to increase the electricity production

R Pop, A Bot, V Rednic and O Raita

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: radu.pop@itim-cj.ro

Abstract. The construction of micro-hydro powerplants are different, they are built according to the location (the level differences between water intake and powerhouse). Depending on location, the differences between construction of micro-hydro powerplants consist in: type of the water intake, pipe and hydraulic turbine. The aim of this contribution is to present the possibility to implement new technical optimization solution for the river flow capture process, in several micro-hydropower plants with different types of water intakes or hydraulic turbines, in order to increase their hydroelectric power production.

Poster T3-14

Optimization of hybrid energy system for residential applications

M S Raboaca[1,2,3], **C Filote**[2], **C Oprea**[3] **and R A Felseghi**[2]

[1]National Research and Development Institute for Cryogenic and Isotopic Technologies-ICSI, Uzinei, No. 4, P.O. Box 7 Raureni,240050, Ramnicul Valcea, Romania.

[2]Faculty of Electrical Engineering and Computer Science, "Ştefan cel Mare" University of Suceava, Universităţii, no.13, 720229 Suceava, Romania;

[3]Technical University of Cluj-Napoca, Memorandumului Street, no. 28, 400114, Cluj-Napoca, Romania;

E-mail: simona.raboaca@icsi.ro

Abstract. A hybrid energy system is an energy system that can supply a building through primary or secondary energy conversion equipment by grid or renewable energy sources. In order to design a hybrid energy system, it is necessary to address the consumer's energy needs as well as the operating strategy. In this context, we define the energy need and optimize the energy produced, the converted energy, the stored energy and the energy consumed by the auxiliary equipment. Actually, in the literature, this problem is addressed for different system configurations. In this paper is a synthetic presentation of this subject. Based on this subject, this paper presents the contributions to the development of specific knowledge regarding the definition of the selection criteria of the energy generating systems to be installed, energy sources, functioning strategies and technical solutions that aim at greater efficiency in the use of renewable energy, but also the reduction of CO_2 emissions in the buildings sector, which accounts for 40% of Europe's primary energy needs.

Poster T3-15

Structural investigation of recycled and vanadium-copper doped materials

M Rada[1], M Zagrai[1], D Cuibus[2], S Macavei[1], R Erhan[3,4], V Bodnarchuk[5] and S Rada[1,2]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies, 400293 Cluj-Napoca, Romania

[2] Physics and Chemistry Department, Technical University of Cluj-Napoca, 400020 Cluj-Napoca, Romania

[3] Physics Department, Institute for Energy Technology, Norway

[4] Department of Nuclear Physics, Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Bucharest - Magurele, Romania

[5] Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russian Federation

E-mail: marius.rada@itim-cj.ro

Abstract. Lead-acid batteries are supplied by a large, well-established, worldwide supplier base and have the largest market share for rechargeable batteries both in terms of sales value and MWh of production. The majority of industrial batteries are used for standby applications to provide secure power for telecommunications, data networks, national security, and a huge range of applications where continuity of the electricity supply is essential.
This work is focused on the recovery of the spent plates from lead acid battery by melt quenching method. This method offers an alternative for the maximum recovery efficiency and the optimization of conductive performances with other oxides which overcomes the limitations of traditional methods. Structural and behavioural investigations of samples in the $xV_2O_5 \cdot 10CuO \cdot (90-x)[4PbO_2 \cdot Pb]$ composition where x=0-20mol % V_2O_5 were performed by XRD, FTIR, UV-VIS and SANS spectroscopies. XRD patterns show the vitroceramic nature of all obtained samples. Small-Angle Neutron Scattering (SANS) investigations on glassceramics samples were carried out at YuMO SANS spectrometer, IBR-2 pulsed reactor. **Acknowledgments**. This paper was financially supported from the MCI, Nucleu-Program, project number PN 19 35 01 01.

Poster T3-16

An overview on the structure of recycled materials from spent lead acid battery and modified with CuO and MnO_2

S Rada[1, 2], L Mihaila[2], A Popa[1], S Macavei[1], M Zagrai[1], M Rada[1], M Suciu[1] and J Zhang[3]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, 400293, Romania
[2] Department of Physics & Chemistry, Technical University of Cluj-Napoca, 400020, Romania
[3] Beijing Synchrotron Radiation Facilities, Institute of High Energy Physics, Beijing, People's Republic of China

E-mail: simona.rada@itim-cj.ro

Abstract. Spent batteries and accumulators can be recycled almost integraly in order to the avoid of the pollution and the recover of the contained materials. The aim of this work was to explore the structure of the system in the $xCuO \cdot 5MnO_2 \cdot (95-x)[4PbO_2 \cdot Pb]$ composition where x=0-30mol%CuO. The transition metal ions, such as manganese and copper ions are interesting due to their good solubility and can exist in a different number of valence states in different glass matrices which leads to semiconducting properties. The samples were prepared by melt quenching method and were used as starting materials the active plates of spent lead acid battery, MnO_2 and CuO powders. Obtained samples were characterized by XRD and SEM analysis and investigations of FTIR, XAS and EPR spectroscopy. The comparative study of data from different techniques shows that the melt quenching method is efficiently to recycle active material from anodic and cathodic car battery plates and to optimize with another oxide. **Acknowledgments.** This work was supported by a grant financed by Romania-China Partnership Cooperation Projects with No. 13 BM / 2018.

Poster T3-17

Test bench for multiple connectors cable harness certification

G Rosca on behalf of INCDTIM ATLAS Group

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: Gabriel.rosca@itim-cj.ro

Abstract. The poster presents a versatile test bench developed for certification of multiple connectors cable harness. Based on PIC 32 Microchip architecture together with software routines, the test bench checks all possible connections within a cable harness assembly for opens, shorts and miss wires. LED's indicate a Pass or Fail and the LCD display listed any faults such as connections failure, short circuits or inversions. The test bench was developed for production certification of the low voltage distribution cables inside the Tile Calorimeter, one of the detectors of the ATLAS experiment at LHC-CERN.

Poster T3-18

CFD modelling of 3D-printed structured sorbents used in Sorption-Enhanced Water-Gas Shift

V Sandu[1], I Dumbrava[1], A M Cormos[1], A Imre-Lucaci[1], C Cormos[1], S N Sluijter[2] and R de Boer[2]

[1] Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Arany Janos 11, 400028 Cluj-Napoca, Romania

[2] ECN part of TNO, Westerduinweg 3, 1755 LE Petten, The Netherlands

E-mail: cani@chem.ubbcluj.ro

Abstract. The attempt to reduce the carbon footprint of existing technologies used in today's society requires solving the challenge that is equipment size and energy consumption associated with carbon removal. Sorption-enhanced water-gas shift combines the water-gas shift reaction with on-site CO2 adsorption, leading to the direct conversion of syngas into high temperature streams of H2 at feed pressure and CO2 at regeneration pressure. 3D printed structured sorbents of hydrotalcite adsorbent material replace the regular packed-bed configurations in SEWGS, as the latter show restrictions regarding flow-rate inside the column, pressure drops and adsorption kinetics. Simulations in COMSOL Multiphysics of the adsorption step in SEWGS, taking into account mass, momentum and heat transport, are used to determine the performance of monolith structures compared to traditional packed-bed columns. Modelling studies show that monolith structures provide an increase in productivity in the case of sorbent-based technologies for carbon capture and storage.

Poster T3-19

Effect of burning temperature on the thermal and mechanical properties of ceramic blocks

M Streza[1], **N Cobirzan**[2], **M Stan**[1], **B Belean**[1] **and G Borodi**[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2]Techical University 400641 Cluj Napoca, Romania

E-mail: mihaela.streza@itim-cj.ro

Abstract. The goal of this work is to investigate the influence of burning temperature on the thermal conductivity and mechanical strength of some ceramics obtained by adding sawdust and sewage sludge as pore additives into the fabrication recipes. The microstructural characterization of basic raw materials (clays) and additives was done by X-ray analysis, their decomposition temperature by TG/DTA technique, and the thermal properties of the resulting samples were obtained by combined infrared lock-in thermography (LiT) and photopyroelectric calorimetry (PPE) in front configuration. The pore morphology was obtained by image processing. Both thermophysical and mechanical properties are influenced by the firing temperature. The higher temperature will lead to a higher thermal conductivity and a higher mechanical strength of the resulting materials. To keep the mechanical properties above the values recomended by the seismic codes, selecting the minimum temperature at which the bricks are fired is critical. It was shown that the firing temperature in the oven must exceed 850^0C, while the precentage of porosity agent can not exceed 12wt%.

Poster T3-20

Microstrip antenna as open resonator for metamaterial used in rectifier antenna efficiency improvement

E Surducan, R Gutt, C Neamtu and V Surducan

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: emanoil.surducan@itim-cj.ro

Abstract. A rectifier antenna (rectenna) is composed of an antenna and a rectifier circuit, operating in a specific electromagnetic frequency range. A stack of a microstrip rectenna and a specific metamaterial can improve the rectenna efficiency. In this case the metamaterial is a periodical structure of resonators manufactured on a dielectric substrate. At the resonant frequencies, the metamaterial increases the dielectric permittivity and electric storage capacity of the dielectric material support. A microstrip rectenna was previously realised and tested. We present here the experimental characteristics of one microstrip antenna, the basic resonator cell in the periodical structure of the metamaterial. For its design, a microstrip spiral configuration and operating frequency bands of 860 - 960 MHz (GSM) and 2.4 - 2.5 GHz (extended WLAN) were chosen. **Acknowledgments.** This paper was financially supported from the MCT, Nucleu-Program, project no PN 19 35 01 01

Poster T3-21

Pseudorandom number generator for sub-milliwatt applications

V Surducan, R Gutt and E Surducan

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: vasile.surducan@itim-cj.ro

Abstract. To generate a pseudorandom number, an initial seed stored in a number of words is required. The seed value has to be modified before each newly generated number. Sub milliwatt hardware requires (start power)–(run algorithm)–(stop power) sequences to conserve the supply energy. Thus, before each stop, the old seed value has to be stored in a non-volatile memory and read at the next start. We present here an ingenious method to implement it without using memory. Our manufactured hardware used for tests has: one low power microcontroller PIC12LF1572, one start button, seven ultra-low power LEDs and four resistors, the assembly is supplied from an electromagnetic harvesting device in 2V…3V range. After each start, the environment temperature is measured and stored in one of the seed words which alter the overall seed value. The electrical performance of the entire device was measured in on and off state. The random generator quality has been computed using chi-square test with random number buckets (400 samples). The entire hardware has a leakage current of less than 0.8μA and draws less than 0.5mA supply during display of ten successive dice symbols. Chi-square test (χ^2=9.2) reveals the feasibility of pseudorandom generation (95% confidence). Non-volatile memory was not needed. Practical demonstration can be seen in the poster session.
Acknowledgments. This paper was financially supported from the MCT, Nucleu-Program, project no PN 19 35 01 01.

Poster T3-22

Reconstruction of raw OCT images

F Toadere and N Tosa

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: florin.toadere@itim-cj.ro

Abstract. An image processing algorithm that improves the quality of raw Optical Coherence Topographic (OCT) images by reducing their blur and noise is presented. The algorithm consists of three steps: first ten raw OCT images of the human eye are blended together. Then the resulting blended image is filtered using an un-sharing mask and an anisotropic filter. Finally, contrast of the filtered image is enhanced. Demonstrative images illustrating a comparison between original raw OCT images and their images reconstruction are presented. Results illustration depicts the ability of the algorithm to reveals fine details that are not visible in the original raw image. **Acknowledgment.** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PPCDI-2017-0010 / 74PCCDI / 2018, within PNCDI III.

Poster T3-23

A model for coherent beam combining of two ultrashort laser pulses

V Tosa and A M M Gherman

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: tosa@itim-cj.ro

Abstract. ELI-NP project has in plan combining two ultrashort pulses (22-25 fs), each of 10 PW power, in order to use the resulting pulse for different experiments. The coherent beam combining (CBC) is difficult to realize experimentally and the resulting field is depending in a complex manner on the power of the two beams, their delay in time, their focusing configuration and their reciprocal direction of propagation. Here we present a model for calculating the field $E(x,y,z,t)$ which result as a combination of two beams propagating under a given angle, each being specified by their pulse energy, duration, direction of polarization, carrier to envelope phase, each being focused independently in a common interaction region. We present the main capabilities of the model, estimate CBC efficiency, and show selected results to demonstrate the usefulness of such calculation for experiments to be performed at ELI-NP facility. Financial support is acknowledged to CNCS-UEFISCDI project RO-CERN 03ELI (PROPW).

Poster T3-24

Absolute intensity calibration and application at BSRF SAXS station

Z Li and F Xie

Beijing Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Science, 100049 Beijing, China

E-mail: lzh@ihep.ac.cn

Abstract. Small Angle X-ray Scattering (SAXS) is a common physical method to characterize the structure of materials on the nanoscale. The absolute scattering intensity contains quantitative information related to the mass and density of materials. In this work, we studied the absolute intensity calibration method with standards, deduced the formulae and developed the calibration scheme. It needs only measuring the standard and the sample under the same conditions, and recording the relative scattering intensity distribution and the transmitted intensity simultaneously for each measurement. In the measurement, the incident beam intensity does not need to be recorded whether it is constant or decaying. The calibration is simple and convenient. We performed the calibration experiments on the 1W2A SAXS station at Beijing Synchrotron Radiation Facility (BSRF) with glass carbon and water as standards. The comparison of the two standards were discussed. It seemed that the glass carbon SRM 3600 performed better. The application on the determination of ovalbumin molecular weight and porosity variation in the pyrolysis process of anthracite verified the validity of the calibration method.

Poster T3-25

Glass-ceramic electrodes for electrochemical energy storage

M Zagrai[1], M Rada[1], R C Suciu[1], S Macavei[1], M E Pica[2], S Rada[1, 2] and A Bot[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Department of Physics & Chemistry, Technical University of Cluj-Napoca, 400020, Romania

E-mail: mioara.zagrai@itim-cj.ro

Abstract. Among various electrochemical energy storage technologies, battery energy storage are the most highly promising and efficient cost-effective solution for a variety of applications including handheld electronic devices, automotive applications and Smart Grids with high stakes for human development, environment, economic growth and sustainable development. In this study we report a new vitreous system having the $15MnO_2$□$85[(100-x)PbO_2$□$xPb]$ composition where x = 0-100 mol % Pb prepared by melt-quenched method. The samples were investigated by X-ray diffraction (XRD), Fourier Transform Infrared (FTIR), UltraViolet-Visible (UV-Vis), Photoluminescence (PL) Spectroscopies and measurements of Cyclic Voltammetry (CV). The XRD analysis indicates the presence of three crystalline phases, namely Pb, PbO and PbO_2. The examination of the IR spectra shows some modifications of the main structural units with the increasing of lead content in the host matrix. Values of the optical band gap energies are smaller than 3eV indicating a semiconductor behavior of the samples. The influence of the sample composition on the luminescent properties of the lead and manganese ions produces modifications of the emission bands intensities. The relationship between their structure and electrochemical properties are strongly dependent on its composition. Our result suggests the applications of the vitroceramic electrodes in the car battery domain. **Acknowledgments**. This paper was financially supported from the MCI, Nucleu-Program, project number PN 19 35 01 01.

Section T4:

Nanostructured Materials - Nanocomposites and Hybrid Materials

Oral T4-1

MIL-101(Cr)'s synthesis by green chemistry

O Grad, G Borodi, M Dan, D Lazar, D Lupu and G Blanita

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: Gabriela.Blanita@itim-cj.ro

Abstract. Metal-organic frameworks (MOFs) are organic-inorganic hybrid crystalline materials which knew an explosive growth due to their exceptional textural properties, and compositional and structural versatilities. The commercial availability of the MOFs dictates their future development and implementation of various applications. An essential step is the development of some synthetic ways to provide MOFs with desired properties, in high purities and yields. Ideally, these methods should be designed, developed and implemented in a sustainable way. A green synthetic method for MIL-101(Cr), one of a most representative metal-organic frameworks, was developed and scaled-up, eliminating the usual additives. The effect of synthetic parameters, such as concentration of reaction mixture, temperature (180-220°C) and reaction time (4-24 hours) on the product quality and properties were investigated in order to optimize it. **Acknowledgements.**This work was supported by a grant of the Romanian National Authority for Scientific Research and Innovation, CNCS - UEFISCDI, project number PN-II-ID-JRP-RO-FR-2015-0025.

Oral T4-2

Tailoring the size, shape and composition of magnetic nanoparticles and clusters for biomedical applications

I Craciunescu[1], G M Ispas[1], S A Porav[1], V Kuncser[2] and R Turcu[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293, Cluj-Napoca, Romania

[2] National Institute of Materials Physics, 405A Atomistilor str., Bucharest-Magurele, Romania

E-mail: izabell.craciunescu@itim-cj.ro

Abstract. Iron oxide and ferrite magnetic nanoparticles were synthesized with various shapes and sizes, including spherical, cubic, hexagonal and octahedral, from high temperature reaction of organic precursor's solution. Tailoring the shapes and sizes of nanoparticles allows controlling a variety of properties that are relevant to many potential applications of magnetic nanoparticles. Shape and composition can be used to control the structural and morphological properties of the nanoparticles and to achieve high packing density in self-assembled magnetic clusters. The optimization of surface properties of the nanoparticles by coating with hydrophobic or hydrophilic layers, along with their unique magnetic properties makes these nanomaterials very promising for applications in biomedicine. In our experiments, we will discuss the specific properties of magnetic nanoparticles and clusters which are directly related to their applications for magnetic hyperthermia therapy. **Acknowledgement.** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0062, contract no. 58 within PNCDI III and project number PN-III-P1-1.2-PCCDI-2017-0769, within PNCDI III.

Oral T4-3

Titanium nitride nanostructured films as an alternative platform for plasmon-enhanced optical processes

C Farcau[1], A M M Gherman[1], A Vladescu[2], A Falamas[1], C Firta[1], R Gutt[1] and V Tosa[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania;

[2] National Institute for Research and Development for Optoelectronics INOE2000, 409 Atomistilor St. RO77125, Magurele, Romania

E-mail: cfarcau@itim-cj.ro

Abstract. Surface plasmons on nanostructured noble metal films provide the means to control and enhance several optical processes, such as light absorbtion and scattering by surfaces, Raman scattering and fluorescence by molecules, photothermal effects, or photocatalysis. Plasmonic platforms usually consist of noble metals Au or Ag, which can impose limitations on their application area. Titanium nitride (TiN) is an alternative plasmonic material, possesing a thermal and mechanical stability better than noble metals, and an optical response similar to that of Au. Here, we fabricate nanostructured TiN films by colloidal lithography, study their optical properties by experiment and simulation, and explore their potential for plasmonics. Specifically, TiN-coated microsphere arrays are fabricated by TiN sputtering on top of self-assembled polystyrene microsphere lattices and are characterized. Their light-induced plasmonic heating, and potential as substrates for surface enhanced Raman scattering are analyzed. Our results contribute to the increasing efforts currently directed towards finding alternative plasmonic materials exhibiting a good plasmonic efficiency complemented by specific characteristics not available in noble metals.

Oral T4-4

Bioinspired hybrid materials for cancer therapy

R Mrówczyński[1], A Jędrzak[1,2] , B F Grześkowiak[1], E Coy[1], K Szutkowski[1], D Maziukiewicz[1], T Jesionowski[2] and S Jurga[1]

[1] NanoBioMedical Centre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3, PL-61614 Poznan, Poland

[2] Poznan University of Technology, Faculty of Chemical Technology, Berdychowo 4, PL-61131 Poznan, Poland

E-mail: radoslaw.mrowczynski@amu.edu.pl

Abstract. Magnetic nanoparticles have drawn a lot of attention as core materials for the preparation of theranostic nanomaterials since they exhibit a synthetic and functional advantage over other classes of nanomaterials. Lately, the biopsied polydopamine has entered the field of nanomedicine as a versatile coating for nanomaterials vesting them photothermal properties. In this talk, we present merging of polydopamine coated magnetic nanoparticles with PAMAM dendrimers and cyclodextrins and their application in combined chemo- and photothermal therapy of liver cancer. In the second part of the lecture, we present the application of polydopamine nanoparticles in gene therapy of glioblastoma multiform which is one of the most aggressive and lethal types of cancer of the central nervous system. Our approach is based on down-regulation of Tenascin-C using RNA interference (RNAi) strategy and nanomaterials as delivery vehicles. The research was financed by The National Science Centre, Poland under project number 2016/21/B/ST8/00477 and by the National Centre for Research and Development under research program LIDER/11/0055/L-7/15/NCBiR/2016.

Oral T4-5

Theoretical investigation of impurity-substituted thermoelectric SiO_2

Y Noda[1], **T Nishii**[2] **and J Onoe**[3]

[1] Department of Materials Physics, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, Aichi 464-8603, Japan

[2] Research & Development Department, Electric Power Development Co., Ltd. (J-Power), 6-15-1 Ginza, Chuo-ku, Tokyo 104-8165, Japan

[3] Department of Energy Science and Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, Aichi 464-8603, Japan

E-mail: noda@mp.pse.nagoya-u.ac.jp

Abstract. A sustainable energy supply system becomes important to keep our good life. On the other hand, one of SDGs (Sustainable Development Goals) is to reduce CO_2 emission for development of our sustainable society, because CO_2 is well known to cause global warming that results in abnormal weather in the world. To solve both issues, we focus on geothermal power plantsbecause they supply electric power stably, have no CO_2 emission upon electric power generation, and are not influenced by weather. Thus, novel thermoelectric materials working under high temperature and high pressure are necessary to develop high-performance geothermal power plants. In this study, we have investigated the energetic stabilities and thermoelectric properties of SiO_2 crystals partly substituted with various kinds of metals using first-principles calculations, and will present the theoretical results.

Oral T4-6

Magnetization dynamics in perpendicularly magnetized media under the influence of an electric field

R A One[1,2], **S Mican**[1], **A Mesaroş**[2], **M Gabor**[2], **T Petrişor**[2], **L Buda-Prejbeanu**[3] **and C V Tiuşan**[1,2]

[1] Babeş-Bolyai University, Faculty of Physics, Cluj-Napoca, Romania

[2] Technical University of Cluj-Napoca, Romania

[3] National Center of Scientific Research, France

E-mail: roxanaalinaone@gmail.com

Abstract. The advances of spintronics towards faster and more energy efficient storage media rely among many other techniques (spin transfer toque and spin orbitronic effects, all optical switching, etc.) on controlling the magnetic anisotropy by using an electric field. Such a voltage controlled magnetic anisotropy (VCMA) yields in superior storage devices, allowing the tailoring of the interest structures in order to increase the storage density. Tackling on this subject, our approach relies the analysis of the magnetization response to a pulsed electric field, as we already have the experimental proof and a set of experimental parameters for this phenomenon. Not only that we sought for optimum conditions in which the applied electric field leads to the magnetization reversal, but we went further into minimizing as much as possible this value. An important aspect we took into consideration is the relation between the coercivity of the ferromagnetic film and the switching probability, so various configurations have been investigated as well as pulse shapes.

Oral T4-7

Specific reaction field in the sub-nm space of one-dimensional uneven structured C_{60} polymer film for CO_2 activation and immobilization

J Onoe[1], **M Nakaya**[1], **S Watanabe**[1] **and Y Kitagawa**[2]

[1] Nagoya University, Department of Energy Science and Engineering, Chikusa-ku, Nagoya, Japan

2 Osaka University, Department of Materials Engineering Science, Toyonaka, Osaka, Japan

E-mail: j-onoe@energy.nagoya-u.ac.jp

Abstract. Immobilization and reuse of CO_2 is one of the urgent tasks for sustaining our global environment. We have recently found that CO_2 can be easily immobilized by reacting with H_2O at room temperature (RT) in the sub-nm space constructed in one-dimensional (1D) metallic uneven structured C_{60} polymer film, even though the reaction cannot take place at RT in gas phase (activation energy E_a: ca. 2 eV). In addition, the reaction did not proceed in the sub-nm space of pristine C_{60} film. These results suggest that not only the sub-nm space but also the framework of the 1D polymer play a specific role for the reaction occurred at RT. First-principles calculations indicate that CO_2 molecule is stuck in between adjacent 1D C_{60} polymer chains at their concave portions, and then H_2O molecule attacks to the CO_2 with bending that remarkably reduces the E_a enough for the reaction to proceed at RT.

Oral T4-8

Modeling of the Grain Size Effects in Nanostructured Ferroelectric Ceramics

L Padurariu, C Enachescu and L Mitoseriu

Faculty of Physics, Al. I. Cuza University of Iasi,11 Bv. Carol I, 700506 Iasi, Romania

E-mail: leontin.padurariu@uaic.ro

Abstract. The role of grain size on the tunability (electric field dependence of the dielectric constant) and the switching properties (polarization dependence on the applied field) in ferroelectric ceramics was studied by an experimental-modeling approach. The model represents an innovative combination between Finite Element Method and Monte Carlo simulations. The Finite Element Method (based on Maxwell equations) was used to describe the inhomogeneity of the local electric field introduced by grain boundaries and electric interaction between local dipoles. The Monte Carlo simulations (based on Landau-Ginzburg-Devonshire theory) were used to describe the domain structure formation and evolution under field. The simulation results were compared with barium titanate ceramics with grain sizes from few μm to 100 nm. A remarkable agreement between the experimental tunability and switching data and the simulation results was obtained when reducing grain size: (i) the linearization of the permittivity dependence on the applied electric field, (ii) the reduction of the effective permittivity and the tunability, (iii) the increase of the coercive field and the tilting degree of the polarization dependence on the applied field (hysteresis loop), (iv) the reduction of the saturation/remanent polarization and hysteresis area. This work was supported by the CNCS-UEFISCDI Project No. PN-III-P1-1.1-PD-2016-1069.

Oral T4-9

Security paper with embedded magnetic nanoparticles

D Buteica[1], I Borbath[2], I V Nicolae[3], R P Turcu[4], O Marinica[5] and V Socoliuc[6]

[1] SC CEPROHART SA, Al.I. Cuza Ave. 3, 810019 Braila, Romania

[2]SC ROSEAL SA, Nicolae Balcescu 5/A, 535600 Odorheiu Secuiesc, Romania

[3] SC DATRONIC-NCIP SRL, Coriolan Baran 6 apt.1, 300238 Timisoara, Romania

[4] National Institute for Research and Development of Isotopic and Molecular Technologies, Donat 67-103, 400293 Cluj-Napoca, Romania

[5] Politehnica University of Timisoara, M. Viteazu Ave. 1, 300222 Timisoara, Romania

[6] Romanian Academy – Timisoara Branch, M. Viteazu Ave. 24, 300223 Timisoara, Romania

E-mail: vsocoliuc@gmail.com, vsocoliuc@acad-tim.tm.edu.ro

Abstract. Multicore-shell Fe_3O_4-SiO_2 magnetic nanocomposites were synthesized at laboratory scale and transferred to micro-pilot production. The nanocomposite powder was dispersed in cellulose pulp and paper was produced by dehydration on a Rapid Kothen machine. Paper with uncoated magnetite particles was also produced for comparison. Manifold characterization of the paper samples is presented. It is shown that using magnetic multicore-shell composites for paper magnetic loading diminishes to almost half the coloring of the paper. The coloring reduction can be further improved by increasing the SiO_2 shell thickness. First instance one sided detection and authentication demonstrator, based on Magnetic Particle Spectroscopy, is presented.

Oral T4-10

Synthesis and Properties of Molecular Bowls of Carbon

M C Stuparu

School of Physical & Mathematical Sciences and School of Materials Science & Engineering, Division of Chemistry and Biological Chemistry, Nanyang Technological University, 21 Nanyang Link, 637371 Singapore

E-mail: mstuparu@ntu.edu.sg

Abstract. Corannulene ($C_{20}H_{10}$) is a bowl-shaped polycyclic aromatic hydrocarbon that can be conveniently imagined as the cap region of fullerene C_{60}. Due to the molecular curvature, its properties differ from the typical properties of planar polycyclic aromatic hydrocarbons. For example, corannulene is electron deficient and can accept up to four electrons. In comparison, large planar polycyclic aromatic hydrocarbons such as pyrene and coronene are electron rich compounds. While, ball-shaped molecules such as fullerene C_{60} can accept up to six electrons. Therefore, corannulene behaves very different from the flat or ball-shaped aromatic systems and represents a unique building block in synthesis of organic materials. In this presentation, we will discuss our synthetic efforts in gaining access to a large variety of corannulene derivatives and their use in construction of functional materials.

Oral T4-11

Chitosan-based biocomposites doped with VIS-NIR sensitive particles

N Tosa[1], F Toadere[1], S Porav[1], C Tudoran[1], A Costea[2], V Cebotari[1,3] and V Tosa[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] University "Politehnica" of Bucharest, Faculty of Electronics, Telecommunications and Information Technology, 1-3 Bulevardul Iuliu Maniu, 061071 Bucharest Romania

[3] Technical University of Cluj-Napoca, Faculty of Materials and Environmental Engineering, 103-105 Bulevardul Muncii, 400641 Cluj-Napoca, Romania

E-mail: nicoleta.tosa@itim-cj.ro

Abstract. This work presents investigations on chitosan-based biocomposites doped with VIS-NIR sensitive particles. Morphological aspects of the biocomposites were corelated with their spectroscopic behaviour. VIS sensitive particles were generated within the chitosan-based films and showed a relative uniform size distribution across the biocompatible matrix. The recorded spectra were used within a spectral image processing algorithm to determine variation of the film hues. The matrix density overcomes the dopants aggregation, whilst its transparency emphasises the dopants colours. Therefore, chitosan-based biocomposites properties recommend them as candidates for phantom in optical coherent tomography investigations. **Acknowledgement.** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PPCDI-2017-0010 / 74PCCDI / 2018, within PNCDI III.

Oral T4-12

Self-Propelled Microbotics for the Removal of Pollutants from Water

R D Webster[1,2]

[1] Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, 21 Nanyang Link, Singapore 637371, Singapore

[2] Environmental Chemistry and Materials Centre, Nanyang Environment & Water Research Institute, 1 Cleantech Loop, CleanTech One #06-10, 637141, Singapore

E-mail: webster@ntu.edu.sg

Abstract. Six different forms of naturally occurring nanoclays (Cloisite 10A, 15A, 20A, 25A, 30B and 93A) were sputter coated with platinum metal to form platinum-Cloisite (Pt-Cloisite) microbotics. The fabricated microbotics were roughly spherical with wrinkled and rough surfaces with the exception of Pt-C25A, which appeared to have a needle-like surface morphology. The average dimensions of each Pt-Cloisite microbotic measured with SEM was found based on the mean of 100 microbotics, and were between 12 - 18 μm. The microbotics were suspended in 5 wt% hydrogen peroxide aqueous solutions containing the organic pesticide, fenitrothion. The microbotics were able to self-propel due to the generation of oxygen gas caused by the catalytic decomposition of hydrogen peroxide by platinum on the surface. The fabricated Pt-Cloisite microbotics were all found to move with fast average velocities ($v > 100$ μm/s). The hydrogen peroxide catalysed self-propelled movement of the microbotics combined with their adsorptive properties led to a substantial decrease in the pesticide concentration, as measured by liquid chromatography - mass spectrometry.

Oral T4-13

Oxide and silicide thin films for thermoelectric devices

L P Zarbo

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: liviu.zarbo@itim-cj.ro

Abstract. The band structure of some oxides and silicides of some transitional metals presents unusual features such as flat bands near the Fermi level. Such flat bands have been associated with improved thermoelectric properties. In order to verify this hypothesis experimentally, and futher search for novel thermoelectric materials, we developed the procedure for the pulsed laser deposition of thin crystalline films of copper and titanium oxides, and iron and chromium silicides. We present the current status of this work, along with our extensive tests of the quality of our films by X-Ray diffraction, scanning electron microscopy, atomic force microscopy, etc.

Oral T4-14

In situ X-ray absorption spectroscopy and its application in nanocatalysts

J Zhang, L Zhang, P F An, C Q Chu and L R Zheng

Beijing Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Science, P.R. China

E-mail:jzhang@ihep.ac.cn

Abstract. X-ray absorption spectroscopy (XAS, also known as X-ray absorption fine-structure, XAFS), in both near (XANES) and post (EXAFS) edge regions, has become a powerful characterization technique in all the fields of nanocatalysts science. Nanocatalysts are complex materials that usually operate at elevated pressures and temperatures. The acquisition of information about how nanocatalysts work and how to rationally design new nanocatalysts, still remains challenging. Here, in situ XAS techniques such as quick scanning XAS and in situ cell are developped. Using several representative examples, we illustrate the role of in situ XAS techniques in the characterization of nanocatalysts. New insights into the catalyst active phase and catalytic mechanism and nanocatalyst synthesis can obtanied via in situ x-ray absorption spectroscopy (XAS).

Poster T4-1

The influence of synthesis methods on the characteristics of porous forsterite ceramics

A Avram[1], M Gorea[1], A Mocanu[1]and M Tomoaia-Cotisel[1,2]

[1] Babes-Bolyai University of Cluj-Napoca, Faculty of Chemistry and Chemical Engineering, Department of Chemical Engineering, Physical Chemistry Center, 11 Arany Janos Str., Cluj-Napoca, 400084, Romania

[2] Academy of Romanian Scientists, Splaiul Independenţei 54, 050094 Bucharest, Romania

E-mail: aavram@chem.ubbcluj.ro

Abstract. The present work focuses on the synthesis and characterization of some porous forsterite ceramics (FCs) and their potential bioactive properties. Nanometric forsterite powders, namely, derived through sol-gel (SG) and solid state (ST) methods, were used for preparing two types of FCs – one with medium and one with high porosity. All samples were thermally treated between 1200 and 1400 ^{0}C. Medium porosity ceramics (with an apparent porosity in the range of: 27-39% for SG, 17-46% for ST) were obtained through pressing into pellets. High porosity ceramics (with an apparent porosity in the range of: 45-53 % for SG, 30-60 % for ST) were obtained through a gel-casting method. Microstructural characterization was performed on all FCs using XRD, FTIR, SEM and SEM-EDX. Biocompatibility was determined by immersion in simulated body fluid (SBF) for 1, 2 and 3 months, leading to a hydroxyapatite formation on the surface of forsterite ceramics as evidenced by XRD, FTIR and SEM-EDX. **Acknowledgement.** Authors thank UEFISCDI for financial support through grant no. 83.

Poster T4-2

New antibacterial systems for biomedical applications

R Balint[1], A Mocanu[1], S Rapuntean[2], E V Cota[1], O Horovitz[1] and M Tomoaia-Cotisel[1,3]

[1] Babes-Bolyai University of Cluj-Napoca, Faculty of Chemistry and Chemical Engineering, Physical Chemistry Center, 11 Arany Janos, Cluj-Napoca, 400084, Romania

[2] University of Agricultural Sciences and Veterinary Medicine of Cluj-Napoca, 3-5 Manastur, Cluj-Napoca, 400372, Romania

[3]Academy of Romanian Scientists, Splaiul Independenţei 54, 050094 Bucharest, Romania

E-mail: ba_reka@yahoo.com

Abstract. The increased resistance of microorganisms to antibiotics has triggered intense research for finding alternatives, such as the synthesis and stabilization of colloidal silver systems with enhanced antimicrobial activity. The current study describes the synthesis of silver nanoparticles in aqueous media via chemically reducing of silver nitrate with different reducing agents in alkaline medium. The obtained nanoparticles were characterized by modern methods of analysis, AFM, TEM, XRD, and UV-Vis spectra. The synthesis and stability of silver nanoparticles, AgNPs, is essential because the release of silver ions determines a very good antimicrobial effect both against gram-negative and gram-positive pathogens. Small AgNPs, by their rapid penetration into bacteria membrane, cause damage to the pathogens and the antibacterial effect is strong. The results obtained open new perspectives for the development of novel materials with biomedical applications. **Acknowledgement:** Authors thank UEFISCDI for financial support through the grant no. 83.

Poster T4-3

Antimicrobial activity of poly lactic acid microspheres loaded with vancomycin

G A Paltinean[1], R Balint[1], A Mocanu[1], S Rapuntean[2], I Petean[1], O Horovitz[1] and M Tomoaia-Cotisel[1,3]

[1] Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Research Center of Physical Chemistry, 11 Arany Janos str., RO-400028, Cluj-Napoca, Romania

[2] University of Agricultural Sciences and Veterinary Medicine of Cluj-Napoca, 3-5, Manastur Str., RO-400372, Cluj-Napoca,

[3] Academy of Romanian Scientists, 54 Splaiul Independentei, RO-050094, Bucharest, Romania

E-mail: ba_reka@yahoo.com

Abstract. Controlled drug release microspheres represent an effective and favorable tool to optimize drug dosage, deliver drug to a special site or prolong the delivery duration, which opens up a novel prospect for tissue engineering. The advantage of microspheres consists in encapsulation of active substances in a biodegradable polymeric matrix having the desired size and minimal side effects. Poly lactic acid (PLA) is a polymer used to successfully obtain microspheres for the transport of drugs like vancomycin (VCM) in the presence of hydroxyapatite (HAP) as carrier with applications in bone tissue engineering. Microspheres obtained from PLA/@HAP/VCM were characterized using modern techniques: SEM and AFM for morphology, control microsphere size, and controlled release of vancomycin using calibration curves on a UV spectrophotometer. The antimicrobial effect was testing on Staphylococcus aureus and Escherichia coli. The scientific results obtained may contribute to the development of controlled release drug delivery systems for biomedical applications, particularly in orthopedic surgery and active implant coatings. **Acknowledgement:** Authors thank to UEFISCDI for financial support through the grant no. 83.

Poster T4-4

Graphene grown by chemical vapor deposition on metal foams

C Banciu, M Lungulescu, A Bara, G Sbarcea, D Patroi and V Marinescu

National Institute for Research and Development in Electrical Engineering ICPE-CA, 313 Splaiul Unirii, 030138, Bucharest 3, Romania

E-mail: cristina.banciu@icpe-ca.ro

Abstract. Graphene presents special properties like chemical stability, optical transparency, high surface area, high mechanical strength, and high carrier mobility. Usually, graphene is obtained by chemical or thermal reduction of graphene oxide. The resulting graphene exhibit severely compromised conductivity due to the existence of defects and oxygen-containing chemical groups, and numerous non-ideal contacts between graphene sheets. The graphene grown by chemical vapor deposition (CVD) on metal foam substrates overcome these problems. The properties of the graphene structures like ultralow density, high surface area, high mechanical strength, electrical conductivity, and optical transparency, make them suitable for different applications: energy storage and energy conversion devices, environmental systems, bioelectronics, oil sorption and filtration. In this paper, we prepare the graphene structures by using nickel and copper foams as substrate in a CVD process with methane as carbon source at 1000°C under ambient pressure. Different deposition times were used in order to determine the influence of deposition time on the thickness of the deposited graphene layer. The obtained graphene were investigated by SEM, XRD and Raman spectroscopy.

Poster T4-5

New chromium doped zirconium lithium borate glasses and glass ceramics

L Pop, M Bosca, E Culea, V Pop, L C Bolundut and P Pascuta

Physics and Chemistry Department, Technical University, 28 Memorandumului, Cluj-Napoca, Romania

E-mail: liviu.bolundut@chem.utcluj.ro, maria.bosca@phys.utcluj.ro,

Abstract. New samples doped with chromium from $x•Cr_2O_3$-(100-x)•[80•B_2O_3-18•Li_2O-2ZrO_2], glass ceramic system were prepared using the melt-quenching technique. XRD, FT-IR and UV-vis investigations were performed to characterize the influence of chromium on the structural and optical properties of the obtained glass ceramics. XRD measurement reveal that the matrix and the sample doped with 0.1 mol% Cr_2O_3 are amorphous containing two halos. If the doping level increase a crystalline phase containing chromium(III) oxide (Cr_2O_3) appears, in the structure of the studied samples. This increase in structural order is confirmed also by the FT-IR data. Infrared spectra confirm also the presence of BO_3 and BO_4 units that build up the glass ceramic network. UV-vis data certified the presence of chromium in valence state 3 as Cr^{3+}.This kind of materials are of interest due to their conductive properties.

Poster T4-6

EPR and magnetic susceptibility investigation of mangan-zinc-borate glasses

R Ștefan[1], L C Bolunduț[2], P Păscuță[2], A Popa[3] and L Pop[2]

[1] University of Agricultural Science and Veterinary Medicine, 3-5 Calea Manastur, 400372 Cluj-Napoca, Romania

[2] Technical University of Cluj-Napoca, 103-105 Muncii Avenue, 400641 Cluj-Napoca, Romania

[3] National Institute for Research and Development of Isotopic and Molecular Technologies, 65-103 Donath, 400293 Cluj-Napoca, Romania

E-mail: liviu.bolundut@chem.utcluj.ro, lidia.pop@phys.utcluj.ro

Abstract. This paper reviews informations related to interactions and microvecinities but also the valence of manganese ions, with emphasis on mangan-zinc-borate oxide glasses. The xMnO(100-x)[45ZnO·55B_2O_3] glasses, where x = 0 - 40 mol%, were manufactured by the melt-quenching technique and investigated by magnetic susceptibility measurements and EPR spectroscopy. Magnetical behaviour of the studied glasses is due to the presence of manganese ions. From EPR measurements, it was identified in the tetragonal or rhombic distorted symmetries and also in the distorted octahedral symmetry the presence of Mn^{2+} ions. The concentration dependence on the line intensity, corresponding to the absorption centred at g~2.0, may suggest the appearance of Mn^{3+} ions for higher MnO content. Magnetic susceptibility measurements sustained the presence of both Mn^{2+} and Mn^{3+} ions, in good agreement with EPR. Also, it was noticed the existence of antiferromagnetic interactions between the manganese ions. This type of materials, doped with transition metal ions, have been widely used in wastewater treatment, catalysis, sensors, supercapacitors, and alkaline and rechargeable batteries.

Poster T4-7

SERS substrate fabricated by the thermal nanostructuring of a gold film on a glass support substrate

R T Brătfălean, B Cozar and C Nuț

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: bratfalean@itim-cj.ro

Abstract. Gold films were deposited on a glass support substrate inside a molecular beam epitaxy ultra-high vacuum installation, which also has facilities for sample heating and sample treatment with accelerated argon ions. Three such samples were fabricated, according to three different fabrication recipes, aiming to identify a fabrication method for a SERS substrate, which should be obtained by the nanostructuring of the deposited gold film which is induced by its thermally-assisted solid-state dewetting process. During the fabrication process the evolution of the sample's topography was monitored by atomic force microscopy and the SERS performance of the fabricated samples was measured using a dedicated Raman Spectrometer and three different concentrations of a standard SERS analyte – Crystal Violet. Our best SERS sample compares well with a commercial SERS substrate and is reusable. **Acknowledgement.** The authors gratefully acknowledge financial support from the Romanian Research and Innovation Ministry through The Core Program 2019-2022.

Poster T4-8

Influence of reaction parameters on the properties of $Zn_xMn_{(1-x)}Fe_2O_4$-nanoparticles synthesized by co-precipitation reaction

A Bunge[1], T Radu[1], G Borodi[1], V Socoliuc[2], A S Porav[1] and R Turcu[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Romanian Academy – Timisoara Branch, Center for Fundamental and Advanced Technical Research, Laboratory of Magnetic Fluids, Mihai Viteazul 24, 300222 Timisoara, Romania

E-mail: alexander.bunge@itim-cj.ro

Abstract. Magnetic nanoparticles have gained widespread interest for applications as different as biomedicine, separation/water purification, catalysis or data storage. While magnetite is probably the most widely used magnetic material due to its high saturation magnetization (compared to other oxides) and relative chemical stability (compared to metals such as Fe and Co), ferrites offer unique properties such as the possibility of a greater variation of magnetic properties and an even better stability against oxidation than magnetite. Manganese zinc ferrite nanoparticles are nontoxic and a partial zinc substitution of ferrite phases can improve saturation magnetization. In order to improve their size and saturation magnetization, a study was made regarding the influence of various reaction parameters on physico-chemical properties (determined by TEM, XPS, XRD and magnetic measurements), which are important for the potential use of the particles in biomedicine, for example for hyperthermia applications. **Acknowledgement.** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0062, contract no. 58, within PNCDI III.

Poster T4-9

Wet mechanical alloying experiment in the manganese-silicon system

V Cebotari[1, 2], T F Marinca[2], F Popa[2], B V Neamțu[2], R Hirian[3] and I Chicinaș[2]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Materials Science and Engineering Department, Technical University of Cluj-Napoca, 103-105, Muncii Avenue, 400641 Cluj-Napoca, Romania

[3] Babeș-Bolyai University, Faculty of Physics, 400084, Cluj-Napoca, Romania

E-mail: Victor.Cebotari@itim-cj.ro

Abstract. For the preparation of the $MnSi_{1.75}$ alloy, wet mechanical alloying was employed, starting from elemental powders. The initial powder mixture was homogenized 15 minutes and then loaded in the milling vial with gridding media and with 2 ml of benzene. Milling experiment was conducted up to 14 hours. The diffraction patterns recorded for the powder milled 2 hours show the start of a solid-state reaction and the formation of MnSi phase and the reduction of crystallite dimension for the elemental powders. The milling up to 4 hours leads to the formation of a small amount of the HMS (Higher Manganese Silicide) chemical compound and the increasing the amount of MnSi phase. After 6 hours of mechanical alloying, the silicon peaks disappear, marking the reaction of the elemental powders. The continuation of mechanical alloying between 6 and 14 hours leads to the reduction of the HMS amount and the increase of the MnSi phase quantity. After 14 hours of mechanical alloying in the powder, only the MnSi phase is present. The heat treatment performed on the mechanically alloyed powder for 14 hours at 1000 ^{o}C does not lead to the formation of the HMS chemical compound. **Acknowledgement.** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PPCDI-2017-0010 / 74PCCDI / 2018, within PNCDI III.

Poster T4-10

High-throughput fabrication of anti-counterfeiting nanopillar-based quick response codes

A Colniță[1], D Marconi[1], I Brezeștean[1,2], R D Pașca[1], L Barbu-Tudoran[1,3] and I Turcu[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Babeș-Bolyai University, Faculty of Physics, 1 Mihail Kogalniceanu, 400084 Cluj-Napoca, Romania

[3] Babeș-Bolyai University, Faculty of Biology, 44 Republicii, 400006 Cluj-Napoca, Romania

E-mail: alia.colnita@itim-cj.ro

Abstract. Quick response (QR) codes are two-dimensional optical labels which can store information instantly readable by an imaging device such as the smartphone camera. They can be used as low-cost anti-counterfeiting elements in order to help companies and consumers to identify the authenticity/traceability of various products. Three dimensional (3D) nanostructured QR codes are a new class of labels with an increased level of security to better support product authentication. Nanoimprint lithography (NIL) was used to fabricate high resolution 3D nanopillar-based QR codes on IPS® flexible substrates suitable as anti-counterfeiting elements in the automotive industry. The QR code comprise a bicolored pattern where one colour is diffractively generated by a set of 300 nm pitch nanopillars and the second colour arise from a set of 400 nm pitch nanopillars. Scanning Electron Microscopy (SEM) images were used to optimize the NIL process imprinting parameters (the intermediate temperatures and pressures). Optimal individual nanopillars with straight sidewalls on large area of the polymeric substrate were visualized when the imprinting temperature slowly decreased in a controlled manner. A good replication of the mold in the thermoplastic substrate is of key importance to an accurate reading of the label. **Acknowledgement**: This work was supported by a grant of the Romanian Ministery of Research and Innovation, CCCDI – UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0387 / 80PCCDI/2018, within PNCDI III.

Poster T4-11

Graphene oxide and reduced graphene oxide obtained from high purity graphite

M Coroș, F Pogăcean, C Socaci, M C Roșu, A Turza and S Pruneanu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: maria.coros@itim-cj.ro

Abstract. We synthesizedhigh quality graphene oxide (GO) and reduced graphene oxide (rGO) from high purity graphite samples. We report the lowest optimum reduction temperature for converting GO to rGO which has been systematically studied using X-ray diffraction spectroscopy (XRD). The effect of particle size of graphite on properties of GO and rGO was also compared. The GO and rGO were characterized using X-ray diffraction spectroscopy (XRD), UV-Vis spectroscopy, Fourier Transform Infrared spectroscopy (FTIR) and Scanning Electron Microscopy (SEM). The efficient oxidation and reduction process of graphite has led to yield highly oxidized GO and high quality rGO which can be used to prepare high quality graphene for future applications. **Acknowledgements**: This work was supported by a grant of Romanian Ministry of Research and Innovation, under NUCLEU Program, project number PN 19 – 35 02 02.

Poster T4-12

Cotton fabrics treated with TiO_2/SiO_2 and TiO_2/SiO_2/reduced graphene oxide nanocomposites

D Cosma[1], A Urda[1], C Socaci[1], M Coros[1], S Pruneanu[1], F Pogacean[1], V Almasan[1], A Turza[1], M C Rosu[1], L Chirila[2] and D Timpu[3]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] National Research & Development Institute for Textiles and Leather, 16 Lucretiu Patrascanu Street, 030508, sector 3, Bucharest, Romania

[3] "Petru Poni" Institute of Macromolecular Chemistry, 41A Grigore Ghica Voda Alley, 700487 Iasi, Romania

E-mail: dragos.cosma@itim-cj.ro

Abstract. In this study, the cotton fabrics were treated with TiO_2/SiO_2 and TiO_2/SiO_2 graphene oxide (10:1 weigth ratio) nanocomposites via a spraying method. XRD, FTIR and UV-VIS spectroscopy have been used to characterize the nanocomposite powders. The self-cleaning activityof the obtained nanocomposite-treated cotton fabrics was evaluated by photo-discoloration processes of coffee and wine stains under visible light irradiation. The colour differences between the treated cotton fabrics and the control were measured via the CIE *L*a*b** coordinates. Results showed that the stains were partially decomposed after 150 minutes of visible light illumination. **Acknowledgments.** This work was supported by a grant of Romanian Ministry of Research and Innovation, CCCDI – UEFISCDI, Project number PN-III-P1-1.2-PCCDI-2017 0743/44PCCDI/2018, within PNCD III.

Poster T4-13

A comparative study of amorphous $Fe_{38.5}Co_{38.5}Nb_7P_{15}Cu_1$ powders obtained by wet and dry mechanical alloys

A Cotai, B V Neamţu, F Popa, T F Marinca and I Chicinaş

Materials Science and Engineering Department, Technical University of Cluj-Napoca, 103-105 Muncii, 400641 Cluj-Napoca, Romania

E-mail: ana_cotai@yahoo.com

Abstract. This work presents a comparativ study of HITPERM alloy prepared by wet and dry mechanical alloying. This class of alloys have excellent soft magnetic properties even at elevated temperatures. The chosen composition for this study was Fe38.5 Co38.5 Nb7 P15 Cu1 was obtained via mechanical alloying (MA) starting from elemental Fe, Co, Cu powders and the ferroalloys of Nb and P. Mechanical alloying experiments were done using a high energy planetary ball mill under Ar atmosphere.The alloy amorphistation was proved by X-ray diffraction investigations (XRD).The thermal stability and the crystallisation kynetic of the amorphous powders were investigated via differential sanning calorimetry (DSC) and in-situ high temperature X-ray diffraction (HT-XRD). **Acknowledgement.** The results presented in this paper were obtained in the framework of the GNaC 2018 ARUT grant number 142, research Contract no. 3028/05.02.2019, with the financial support of the Technical University of Cluj-Napoca

Poster T4-14

Spectroscopic study of the interaction between phycocyanin and metal nanoparticles

C Firta[1,2], A Falamas[1], C Farcau[1] and S Porav[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Babeş-Bolyai University, Faculty of Physics, 1 Kogalniceanu Street, 400084, Cluj-Napoca, Romania

E-mail:cfirta@itim-cj.ro

Abstract. Phycocyanin is a pigment binding protein present in the light-harvesting complexes of cyanobacteria and red algae. The pigments are responsible for light harvesting, while the proteins are determining the orientation and the conformation of the complexes, in order to maximize light absorption and energy transfer to the photosynthesis apparatus. Phycocyanin has many applications as a natural colourant in cosmetic and food industry, as a bioactive molecule in pharmaceutical industry and recently as an enhancer for light harvesting in solar cells. In this study we investigate the interaction between phycocyanin and metal nanoparticles. The light harvesting antennas were extracted using size-exclusion chromatography, from the cyanobacteria strain (Arthrospira platensis AICB49). SERS (Surface enhanced Raman scattering) is an ultrasensitive, non-destructive technique that enables label-free detection of molecules and also provides structural information about the analyte. We present preliminary results based on UV-VIS, fluorescence, Raman and SERS spectroscopy for metal nanoparticles functionalized with phycocyanin.

Poster T4-15

Study on the correlation of PAH's content in soil and air with the concentration of PAH's in leaves and flowers

V Băbălău-Fuss[1,2], M Roman[1], A Moldovan[1,3], A Becze[1] and M Tofană[2]

[1] INCDO-INOE2000, Research Institute for Analytical Instrumentation, ICIA Cluj-Napoca Subsidiary, 400293 Cluj-Napoca, Romania,
[2] University of Agricultural Sciences and Veterinary Medicine Cluj-Napoca, 400372 Cluj-Napoca, Romania
[3] Technical University, Faculty of Materials and Environmental Engineering, 103 - 105 Muncii Bulevard, 400641, Cluj-Napoca, Romania

E-mail: anca.naghiu@icia.ro

Abstract. PAH's are a group of hydrocarbons that contain two or more aromatic rings and are ubiquitous found in nature. The European Union regulates concentrations of PAHs in air, water, soil and food due to their carcinogenicity or genotoxicity properties. The aim of the study was to correlate the PAH's content in soil and air with the content in flowers from *Prunus spinosa* (blackthorn) and leaves from *Rosa canina* (dog rose). Samples of soil, air, leaves and flowers were taken in spring time from Cluj County area. Hexan was used for the extraction of samples and HPLC with FLD for analysis of naphthalene, acenaphthene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, benz[a]anthracene, chrysene, benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[a]pyrene, indeno[1,2,3,c,d]-pyrene, dibenz[a,h]anthracene and benzo[g,h,i] perylene. For the extraction of flowers and leaves an Accelerated Solvent Extraction (ASE) system was used. The average value of total PAH's found in the soil samples was 51,34 µg/kg. There was positive correlation between higher levels of PAH's found in air and the content of PHA's in leaves and flowers.

Poster T4-16

Materials based on poly(benzofurane-*co*-arylacetic acid) for the removal of Crystal Violet dye from aqueous solutions

I V Ganea[1,2], A Nan[1] and R Turcu[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Faculty of Environmental Science and Engineering, "Babeș-Bolyai" University, 30 Fântânele, 400294 Cluj-Napoca, Romania

E-mail: iolanda.ganea@itim-cj.ro

Abstract. Dyes are widely used in various industries such as the textiles, paper and plastics, pharmaceutical, food, cosmetics or dyestuffs. Thus, synthetic dyes are one of the major water and soil pollutants released into the environment. Crystal violet (CV) is a type of synthetic dye with complex organic structure, often present in industrial wastewaters due to its intensively use in human and veterinary medicine as a biological stain, bacteriostatic or antimicrobial agent and as a textile dye in textile processing industries. However, CV is regarded as a biohazard substance, because is persistent, acts as a mitotic poison, is potentially carcinogen and clastogene and promotes tumour growth. The current study focuses on the removal of CV from aqueous solutions by applying materials based on poly(benzofurane-*co*-arylacetic acid) (PBAAA) in different batch adsorption experiments. The new type of materials was characterized by FTIR, SEM, TEM, VSM and X-ray photoelectron spectroscopy. The magnetic nanoparticles can be well dispersed in water and easily magnetically separated after adsorption. The effects of various parameters such as initial dye concentration, pH, dosage of adsorbent and contact time have been investigated in order to find the optimum adsorption conditions. **Acknowledgements.** This work was supported by Core project PN-19-35 No. 36N/13.02.2019.

Poster T4-17

The influence of annealing temperature on the Cu_3SbSe_4 phase formation, in thin films deposited by PLD

S Garabagiu, R Gavrea, G Borodi and D Marconi

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: sorina.garabagiu@itim-cj.ro

Abstract. Copper-based chalcogenides are non-toxic, abundant compounds for thermoelectric applications. Cu_3SbSe_4 is a p-type semiconductor, with a narrow band-gap, and a large thermopower. Nanostructuring (in the form of thin films) is a method to improve the thermoelectric properties of the materials. In this case, thin films of Cu_3SbSe_4 have been fabricated by Pulsed Laser Deposition (PLD), from a Cu_3SbSe_4 target. Depositions performed at high temperatures (above 250˚C) result in the formation of Cu_3SbSe_3. With the same deposition parameters, at room temperature, amorphous films are formed. By annealing these amorphous films, the required Cu_3SbSe_4 crystallographic phase has been obtained. The influence of the annealing temperature on the crystallographic phase of these thin films has been assessed. **Acknowledgements**. The authors acknowledge financial support from the Romanian National Authority for Scientific Research and Innovation, through Core Program, Grant No. PN 19 35 02 01. This work was supported through the infrastructure obtained in the project Centre of Advanced Research and Technology for Alternative Energies – CETATEA – 623/11.03.2014.

Poster T4-18

Local electric field enhancement in gold nanoparticles for SERS applications

A M M Gherman and V Tosa

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: maria.gherman@itim-cj.ro

Abstract. When metal nanoparticles (NPs) are in close proximity in an external electromagnetic field, one observes a local field enhancement at the NPs external surface. This electric field amplification founds applicability in surface enhanced Raman spectroscopy (SERS), due to the fact that the dominant role for enhancing the SERS effect is attributed to the electromagnetic mechanism. One way in which the local field may be intensified is by modifying the metal NPs morphology. In this work, mathematical modelling is used to investigate the electric field enhancement in various configurations and shape of the gold nanoparticles (GNP) that are placed on a glass substrate. The influence of the substrate, GNP dimensions, as well as the critical role of the distance between them is investigated. The simulations solve the electromagnetic field propagation problem using a finite element method in 2D and 3D geometries.

Poster T4-19

Hierarchical MOF/γ-Al_2O_3 composites: preparation and characterization

O Grad, M Mihet, M D Lazar and G Blanita

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: oana.grad@itim-cj.ro

Abstract. Metal-organic frameworks (MOFs) are one of the most discussed materials of the last decade. The particular interest in MOF materials is due to their modularity, ultrahigh surface area, organic-inorganic hybrid composition, crystalline nature and tunable porosity. In order to facilitate the realistic applications, it is desirable to develop new synthetic methodologies of new multifunctional MOFs composites which exhibit new properties and that are superior to those of the individual components. In this sense, the controllable integration of MOFs into different structured supports is of the highest importance. Therefore, the aim of this work is the synthesis and characterization of MOFs/γ-Al_2O_3 composites. The influence of different parameters (reaction temperature, synthesis duration, support granulation, reactants/alumina ratio) on the nature and the quality of the composites.

Poster T4-20

Magnetic nanocomposite based on half-metals and semiconductors: structural, microstructural and magnetic properties

I O Pana, S Gutoiu, A Stegarescu, M L Soran, C Leostean, S Pintea, O Opris and M Suciu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: simona.gutoiu@itim-cj.ro

Abstract. Different types of magnetic nanoparticles composites can be designed as multifunctional platforms with controllable magnetic properties, thus being able to facilitate their use in different applications. Moreover, the interface interactions between different components can greatly improve the performance of the multi-components system and even generate new synergetic properties. In this work new nanocomposite systems based on magnetic nanoparticles of half-metallic type coated with semiconducting materials are presented. In case of half metallic ferromagnets, the spin–up (majority) and spin-down (minority) conduction bands are split such that the Fermi level is situated in the upper unfilled minority band. Here we successfully obtained FePt@SiO_2 and CoPt@SiO_2 nanocomposites by a simple chemical deposition method. The elemental composition of materials was determined by XPS measurements, the structure and microstructure was checked by XRD and TEM analyses. The magnetic properties were investigated by using VSM magnetometry methods. **Acknowledgements**. This work was carried out through the Core Programme, developed with the support of MCI, project no. PN19 35 02 03.

Poster T4-21

Surface functionalization of textile materials via combined ultrasound/gamma irradiation

O Capraru[1], M Constantin[1], C Herman[1], L Chirila[2], M-C Rosu[3], I Stanculescu[1], D E Radulescu[2] and D M Radulescu[2]

[1] Horia Hulubei National Institute for Physics & Nuclear Engineering, Reactorului 30, 077125 Magurele, Romania

[2] National R&D Institute for Textile & Leather, 16 Lucretiu Patrascanu, 030508, Bucharest, Romania

[3] National R&D Institute of Isotopic and Molecular Technologies, 67-103 Donat Street, 400293, Cluj-Napoca, Romania

Email: istanculescu@nipne.ro

Abstract. The aim of this study was to functionalize the textile materials (100% polyester and 50% polyester / 50% cotton fabrics) with TiO_2:Ag and TiO_2:Ag-thermally reduced graphene oxide (TRGO) nanocomposites by a combined treatment of ultrasound and Co-60 gamma radiation (dose of 5 kGy). Polyfunctional acrylic monomers as additives for enhancing radiation crosslinking were used. The functionalized fabrics were characterized by Attenuated Total Reflection–Fourier Transform Infra-Red (ATR-FTIR) and Scanning Electron Microscopy (SEM) measurements. The photocatalytic efficiency of functionalized textile materials was investigated by the degradation of methylene blue (MB) under ultraviolet (UV) irradiation. The antibacterial activity of functionalized textile materials against *S. Aureus* and *P. Aeruginosa* was qualitatively determined by disc diffusion method. The experimental results can be useful to promote the obtained textile materials as multifunctional fabrics in a range of applications.

Poster T4-22

Structural and microbiological characterization of gamma irradiated leather

C Herman[1], C Gaidau[2], M Constantin[1], M Stanca[2], O Capraru[1] and I Stanculescu[1,3]

[1] Horia Hulubei National Institute for Physics and Nuclear Engineering, Dept IRASM, 30 Reactorului Str, 077125 Magurele, Ilfov, Romania

[2] National Research and Development Institute for Textiles and Leather (INCDTP), Leather and Footwear Research Institute (ICPI), Str. Ion Minulescu Nr. 93, Sector 3, 031215 Bucharest, Romania

[3] University of Bucharest, Dept of Physical Chemistry, Regina Elisabeta Bld 4-12, 030018 Bucharest, Romania

E-mail: istanculescu@nipne.ro

Abstract. Experiments were carried out with the purpose of obtaining new improved properties and prolong the life of the finished product, the biocide and collagen crosslinking effects of gamma irradiation being well known. Leather materials in different stages of the tanning process where irradiated with doses from 1 to 100 kGy to elucidate their behaviour under gamma radiation. Animal hides were also irradiated, for preservation purpose and to reduce the processing time and costs in the manufacturing process. Decontamination treatments using gamma radiation were carried out in the middle of tanning process with the objective of lowering the waste water and harmful substances used. To enhance the antimicrobial properties of the finished leather products, nanoparticles of Ag+ in chitosan and PVP were applied on leather materials and combined with gamma radiation treatments. The functionalized leather materials were inoculated with *Staphylococcus aureus* and *Pseudomonas aeruginosa* to check their antimicrobial activity. Nanoparticles and gamma radiation functionalization treatment was confirmed by SEM imaging, DSC and FTIR analysis.

Poster T4-23

Study of the Interphase Exchange Coupling in $Nd_2Fe_{14}B$/α-Fe Magnetic Nanocomposites Annealed around Fe α/γ Transition Temperature

R Hirian[1], L Barbu-Tudoran[2,3], O Isnard[4] and V Pop[1]

[1] Faculty of Physics, Babeş-Bolyai University, Cluj-Napoca, RO-400084 Romania

[2] INCDTIM, Cluj-Napoca, RO-400293 Romania

[3] Electron Microscopy Center, Faculty of Biology & Geology, Babes-Bolyai University, RO-400006, Cluj-Napoca, Romania

[4] Institut Néel, CNRS / Université Grenoble Alpes, 25 rue des martyrs, BP 166X, 38042 Grenoble, Cédex 9, France

E-mail: HIRIAN.Razvan@ubbonline.ubbcluj.ro

Abstract. Hard-Soft Exchange coupled nanocomposite magnets rely on a precise control of both structure and microstructure for the constituent phases. In $Nd_2Fe_{14}B$+10wt%α-Fe magnetic nanocomposites obtained through mechanical milling, the nanostructure refinement is achieved by annealing for a short duration. This work builds upon previous results in two ways: (i) increasing rapid annealing temperature and rate, (ii) taking advantage of the Fe α/γ transformation in order to limit the growth of the soft phase crystallites. Annealing was performed at temperatures between 800 °C and 950 °C under purified He gas for durations between 38 s and 65 s. The structure and microstructure of the nanocomposites was studied trough XRD and SEM while their magnetic properties and the effectiveness of the interphase exchange coupling were studied using demagnetization curves (±10 T) and *dM/dH* plots.

Poster T4-24

Bioinspired nanoplatform based on dendrimers grafted to the polydopamine coated magnetic nanoparticles for combined cancer therapy

A Jędrzak[1,2], B Grześkowiak[1], E Coy[1], S Jurga[1], T Jesionowski[2] and R Mrówczyński[1]

[1] NanoBioMedical Centre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3, PL-61614 Poznan, Poland

[2] Poznan University of Technology, Faculty of Chemical Technology, Berdychowo 4, PL-61131 Poznan, Poland

E-mail: radoslaw.mrowczynski@amu.edu.pl

Abstract. Current development of nanotechnology influences on a design and a synthesis of novel and more efficient drug nanoplatforms for medicine, especially in cancer treatment. The application of specific components like PAMAM dendrimers is a prominent topic in cancer therapy due to their internal cavities, and modifiable surface functionality that renders them as an interesting drug delivery carrier. The other most commonly used material in cancer treatment are magnetic nanoparticles of iron oxide. In particular, the magnetite has drawn a lot of attention since they are biocompatible, nontoxic, size/shape-tunable and high surface/volume ratio and allow easy separation from mixtures by an external magnetic field. Moreover, magnetite can be used as contrast agents in nuclear magnetic resonance imaging. Further, polydopamine coated magnetite exhibit high photothermal properties and they are recently extensively investigated in cancer treatment. Here we present, the PAMAM dendrimers grafted to the polydopamine coated magnetic nanoparticles as an attractive and advanced theragnostic tool for dual chemo- and photothermal therapy. Obtained nanocarriers were characterized by means of TEM, zeta potential, FT-IR, XPS, magnetic tests and MRI. Further, the results regarding drug loading and release profile will be discussed as well as their application *in vitro* arranged HepG2 liver cancer cells.

Poster T4-25

Synthesis and characterization of MWCNTs decorated with TiO_2:Cu nanoparticles

C Leostean, O Pana, M Stefan, A Popa, D Toloman, S Macavei and L Barbu-Tudoran

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: cristian.leostean@itim-cj.ro

Abstract. In this paper we report a simple strategy for decoration of MWNTs with TiO_2:Cu nanoparticles by a polymer wrapping-technique that is non-invasive, and does not introduce defects to the structure of CNTs. Due to the unique electronic and physical properties of the MWCNTs, the decoration of MWCNTs with TiO_2 can induce interesting charge transfer and enhance the photocatalytic activity of TiO_2. Also, recent studies have reported the improvement of the photocatalytic activity of TiO_2 by transition metal doping. At a constant MWCNTs : TiO_2 ratio, the Cu doping concentration influence on the composite properties was studied. The composites were characterized by using XRD, RES, TEM and HRTEM, XPS and UV-Vis Spectroscopy. The photocatalytic activity of the nanocomposites was evaluated by photodegradation of Rhodamine B (RhB) in a Laboratory-Visible-Reactor system with a 400 W halogen lamp (Osram) which emits in visible range. The results revealed that by adjusting the composition of components, one can control the decoration efficiency and, by consequence the application areas of these composite nanoparticles.

Poster T4-26

Pulsed laser deposition of ZnO/FePt thin films on Mg (100) substrates

S Macavei, O Pana, M Stefan, D Toloman, A Popa, C Leostean and L Barbu-Tudoran

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: sergiu.macavei@itim-cj.ro

Abstract. Ordered $L1_0$ FePt phase is a promising candidate for applications including biomaterials, permanent magnets, and spintronic devices of nanoscale devices due its large magnetocrystalline anisotropy. FePt thin films were grown on Mg (100) using PLD technique in different deposition conditions. The deposition parameters were adjusted by investigating the structural characteristics by X-ray diffraction, while the morphology was evidenced using SEM microscopy. The best deposition parameters were $P=3 \times 10^{-6}$ mbar, 1200 pulses at 10 Hz and the substrate temperature was 450 ◦C. The magnetic properties were measured by VSM magnetometery with in-plane and out of plane configuration. The exchange coupling behaviour between top ZnO and bottom FePt layer was evidenced by first derivative of the demagnetization curve.

Poster T4-27

High quality anti-counterfeiting labels fabricated on flexible thermoplastic substrates using nanoimprint lithography

D Marconi[1], A Colniță[1], I Brezeștean[1,2], R D Pașca[1], L Barbu-Tudoran[1,3], I Kacso[1] and I Turcu[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Babeș-Bolyai University, Faculty of Physics, 1 Mihail Kogalniceanu, 400084 Cluj-Napoca, Romania

[3] Babeș-Bolyai University, Faculty of Biology, 44 Republicii, 400006 Cluj-Napoca, Romania

E-mail: daniel.maconi@itim-cj.ro

Abstract. State-of-the-art anti-counterfeiting technology is of high interest for both of manufacturers and buyers. Existing anti-counterfeit technologies have some disadvantages such as high cost, complex fabrication process and operation. Nanoimprint lithography (NIL) is an emerging cost-effective patterning technique, suitable to fabricate high throughput, high-resolution and low-cost nanostructured surfaces. It consists in the mechanical patterning of a wide range of materials by using a hard mold with 3D nanoscale features. This report illustrate the excellent capability of the thermal NIL technique for fast, high-throughput fabrication of well-defined quick response (QR) codes on several flexible and transparent substrates (polycarbonate– PC, poly(methyl methacrylate) – PMMA and Cyclic olefin copolymer - TOPAS and ZEONOR sheets). The QR codes are based on selective reflective surfaces made of 3D nanopillars with 300 nm and 400 nm pitch, obtained through the NIL technique. The fabricated QR codes selectively reflect light on two different wavelengths (magenta and yellow respectively) corresponding to the two mentioned pitches. The transition glass temperatures of the flexible polymeric substrates were assessed by Differential Scanning Calorimetry (DSC). Each imprinted polymeric substrate was evaluated using SEM technique and the temperature, pressure and imprinting time used in NIL process were optimized for a precise replication of the mold. **Acknowledgement:** This work was supported by a grant of the Romanian Ministery of Research and Innovation, CCCDI – UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0387 / 80PCCDI/2018, within PNCDI III.

Poster T4-28

Cotton fabrics with improved fire retardant protection

A O Mateescu[1], G Mateescu[1], I Burducea[1], P Mereuta[1], A Urda[2], D Cosma[2], M C Rosu[2], L Chirila[3], A Popescu[3], D M Radulescu[3], D E Radulescu[3] and G C Constantinescu[3]

[1]"Horia Hulubei" National Institute for Research and Development in Physics and Nuclear Engineering, 30 Reactorului Street, 077125, Magurele, Romania

[2] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[3]National Research & Development Institute for Textiles and Leather, 16 Lucretiu Patrascanu Street, 030508, sector 3, Bucharest, Romania

E-mail: amateescu@niham.nipne.ro

Abstract. Aqueous dispersions of SiO_2, N-doped TiO_2 and SiO_2/N-doped TiO_2 nanoparticles were used to deposit coatings onto cotton fabric surfaces via padding method. An additional layer of C/Cu/Ag was applied on nanoparticle-modified cotton fabrics by DC magnetron sputtering. The resulting coating was assessed by Scanning Electron Microscopy (SEM), Rutherford Backscattering Spectrometry (RBS) and optical measurements. The fire retardant tests according to the specific standards showed that the C/Cu/Ag layer improved the flame-retardant properties of the obtained cotton fabrics. **Acknowledgments.** This work was supported by a grant of Romanian Ministry of Research and Innovation, CCCDI – UEFISCDI, Project number PN-III-P1-1.2-PCCDI-2017 0743/44PCCDI/2018, within PNCD III.

Poster T4-29

Surface characterization of treated cotton fibers by atmospheric pressure plasma

G Mateescu[1], A O Mateescu[1], I Burducea[1], P Mereuta[1], L Chirila[2], A Popescu[2], D M Radulescu[2], D E Radulescu[2], G C Constantinescu[2], A Urda[3], D Cosma[3], M Coros[3], C Tudoran[3] and M C Rosu[3]

[1]"Horia Hulubei" National Institute for Research and Development in Physics and Nuclear Engineering, 30 Reactorului Street, 077125, Magurele, Romania

[2]National Research & Development Institute for Textiles and Leather, 16 Lucretiu Patrascanu Street, 030508, sector 3, Bucharest, Romania

[3] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: mateescu@nipne.ro

Abstract. The surface of cotton fibers was modified by atmospheric pressure plasma treatment using helium, nitrogen and argon as working gases. We used a laboratory made experimental plasma treatment system, based on a newly designed plasma applicator head. The plasma-treated cotton fibers were characterized by SEM observations, optical reflectance and wettability measurements. Atmospheric pressure plasma treatment can impart desired functional characteristics to the fibres substrate without modification of bulk properties of textiles. **Acknowledgments.** This work was supported by a grant of Romanian Ministry of Research and Innovation, CCCDI – UEFISCDI, Project number PN-III-P1-1.2-PCCDI-2017 0743/44PCCDI/2018, within PNCD III.

Poster T4-30

Effect of the electron-phonon interaction on the transport properties of a quantum dot connected to Majorana bound states

L Máthé[1,2], D Sticlet[1] and L P Zârbo[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Faculty of Physics, Babeş-Bolyai University, 1 Kogalniceanu, 400084 Cluj-Napoca, Romania

E-mail: levente.mathe@itim-cj.ro

Abstract. We theoretically study the electronic transport properties of a quantum dot attached to two Majorana bound states. The Majorana bound states are located at the ends of a topological superconducting loop that is threaded by a magnetic flux. The dot is also connected to two metallic leads which measure the current through the junction. We consider the interaction of the localized electrons in the quantum dot with a single optical phonon mode in order to analyze the effect of inelastic scattering in such systems. The electron-phonon interaction is treated within the canonical transformation. We calculate the phonon part of Green's function at zero and finite temperatures. We employ the equation of motion technique in order to calculate the retarded Green's function for the dot by taking into account the electron-hole contribution. A formula for the differential conductance and differential shot noise is deduced.

Poster T4-31

Ni@MIL-53 and Ni@MIL-53/Al_2O_3 catalysts: comparative performance in the methanation of CO_2

M Mihet, O Grad, G Blanita, L Barbu-Tudoran and M D Lazar

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: maria.mihet@itim-cj.ro

Abstract. The reaction mechanism of the CO_2 methanation process, also known as the Sabatier process, involves the activation of reactants by adsorption and dissociation either on the metal sites (H_2), or on the support (CO_2), with the subsequent interaction between activated species at the metal – support interface. In this context, metal-organic frameworks (MOFs) might be a viable alternative as catalytic supports considering that (i) enhancement of the hydrogen adsorption capacity could be achieved due to their very large surface areas, which ensures an increased metal dispersion on the support, while (ii) enhancement of the CO_2 adsorption capacity could be achieved due to their tunable porous structure and structural diversity. We report on the use of Ni(10wt.%)@MIL-53 and Ni(10wt.%)@MIL-53-Al_2O_3 as catalysts in the methanation of CO_2 at temperatures below 350°C. MIL-53/Al_2O_3 obtained by macrostructural templating on alumina pellets has the advantage of enhanced chemical and mechanical stability as compared to MIL-53 alone, as well as the possibility of being easier to handle within the catalytic activity experiments. Ni based catalysts were prepared by a modified 'double solvent' method, and were characterized structurally (XRD, BET, TEM-EDX), morphologically (SEM), and functionally (H_2-TPD, CO_2-TPD).

Poster T4-32

Nanodevices, nanorobots and nanomachines for pharmaceutical and biomedical applications

M Tertis[1], **A Cernat**[1], **C Cristea**[1] **and S Mirel**[2]

[1] Department of Analytical Chemistry, Faculty of Pharmacy, Iuliu Hatieganu University of Medicine and Pharmacy, 400021Cluj-Napoca, Romania

[2] Department of Medical Devices, Faculty of Pharmacy, Iuliu Hatieganu University of Medicine and Pharmacy, 400021 Cluj-Napoca, Romania

E-mail: smirel@umfcluj.ro

Abstract. In recent years, the latest approaches in the pharmaceutical field and personalized medicine began to use new technologies and nanodevices for diagnosis and treatment monitoring. Nanorobots and nanomachines are used in heterogeneous domains such as drug delivery, sensing, detoxification, and even in surgery as to improve health care and to address issues difficult to solve by conventional methods. The growing interest toward those nanotechnologies is justified by the performances reported so far. This review will present the latest achievements in nanodevices, nanorobots and nanomachines design targeting pharmaceutical and biomedical applications.

Poster T4-33

CO_2 reduction using porous silica from fly ash waste

M Miricioiu, V C Niculescu, F Bucura and M Constantinescu

National Research and Development Institute for Cryogenics and Isotopic Technologies – ICSI Rm. Valcea, 4th Uzinei Street, 240050 Ramnicu Valcea, PO 7 Raureni, Box 7, Valcea, Romania

E-mail: marius.miricioiu@icsi.ro

Abstract. The CO_2 emissions have been related to climate change, this phenomenon having significant global consequences in both short and long term. Regarding the reduction of CO_2 emissions, the membrane technology attracted enormous attention, but no so much the technology which uses unconventional membranes based on silica obtained from fly ash. The silica was used as filler in the synthesis of mixed membranes with polymer matrix for CO_2 reduction. The scanning electron microscopy revealed a good compatibility between the two phases even at high fillers loadings as 25 wt.%, the resulted membranes being free of gaps. Also, the thermal gravimetric analysis highlighted the thermal stability of the membranes. The gas testing of obtained membranes for emissions reduction applications showed enhanced CO_2 permeability at ambient condition and 1 bar feed pressure, without a significant drop in CO_2/N_2 selectivity even at higher pressure, comparing with neat polymer membrane. The effect of temperature and pressure on membrane performance was investigated. In the case of the 25 wt.% membrane, the CO_2 permeability slightly increased with the pressure increasing up to 9 Barrer while the CO_2/N_2 selectivity remained almost constant.

Poster T4-34

Core-shell nanoparticles based on poly(benzofuran-*co*-arylacetic acid)-peptide conjugates for radionuclides immobilization

A Nan[1], E L Chilug[2], D Niculae[2], G Manda[3] and R Turcu[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, 30 Reactorului, Măgurele, Romania

[3] "Victor Babes" National Institute of Pathology, 99-101 Splaiul Independenţei, 050096 Bucureşti, Romania

E-mail: alexandrina.nan@itim-cj.ro

Abstract. Radiation therapy is an effective cancer treatment option in conjunction with chemotherapy and surgery. With recent advances in nanoscience and nanotechnology, there is great interest in developing nanomaterials as multifunctional carriers to deliver therapeutic radioisotopes for tumour targeted radiation therapy, to monitor their delivery and tumour response to the treatment. The combination of the size-dependent properties of nanomaterials with radioisotopes is emerging as a novel tool in nanomedicine. We report here a polymer which proved, on the one hand, a very good coating for various types of nanoparticles and on the other hand, is an excellent linker for covalent binding of peptides. These novel core-shell nanoparticles are used as a chelate for radionuclides. The final nanostructures where structurally and morphological investigated. **Acknowledgment.** This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0769, contract no. 64, within PNCDI III.

Poster T4-35

Mesoporous silica obtained from rice husk ash for efficient removal of dyes from wastewater

V Niculescu, M Miricioiu, A Soare, A Marinoiu and E David

National Research and Development Institute for Cryogenics and Isotopic Technologies – ICSI Rm. Valcea, 4th Uzinei Street, 240050 Ramnicu Valcea, Valcea, Romania

E-mail: violeta.niculescu@icsi.ro

Abstract. Organic dyes are intensively used in food technology, leather tanning, textile dyes, paper, etc, resulting large amount of so-called coloured wastewater. Many of these dyes have toxic or carcinogenic effects, causing serious damages on aquatic organisms and human being as well. At this moment, the adsorption method is considered the most suitable for removing and recycling the dyes in wastewater. The mesoporous materials have become effective adsorbents own to their unique structures and characteristics such as huge surface areas, high pore volumes, relatively even distributions of pore sizes, surfaces enriched with unsaturated groups and orderly long-range structures. The mesoporous silica nanoparticles were prepared using rice husk ash as silicate source, followed by a hydrothermal method. The mesoporous silica was characterized by UV-VIS, FTIR, SEM and BET surface area, pore volume and pore size distribution measurements. The materials showed highly efficient and rapid adsorption properties for dyes such as rhodamine or Nile blue. The results showed that the adsorption is mainly controlled by electrostatic interactions and hydrogen bonding between the dyes and the mesoporous silica.

Poster T4-36

Chokeberry anthocyanins localization and visualization enhancement via Naturstoff reagent A in B16-F10 melanoma cell line

M Nistor[1], D Rugină[2], M Focșan[3], M Cenariu[2], A Pintea[2] and C Socaciu[1]

[1] University of Agricultural Sciences and Veterinary Medicine, Faculty of Food Science and Technology, 3-5 Calea Manastur Street, Cluj-Napoca, Romania
[2] University of Agricultural Sciences and Veterinary Medicine, Faculty of Veterinary Medicine, 3-5 Calea Manastur Street, Cluj-Napoca, Romania
[3] Babeș-Bolyai University, Faculty of Physics, 1 Mihail Kogalniceanu Street, Cluj-Napoca, Romania

E-mail: nistor.madalina@usamvcluj.ro

Abstract. Anthocyanins are bioactive compounds with protective properties against different types of cancer, including melanoma. Currently, there is no evidence to what extent anthocyanins are taken up by the melanoma cells. In this context, our aim was to determine cellular concentration and distribution of the anthocyanins in melanoma B16-F10 cells. Anthocyanins were extracted from chokeberries, purified through the SPE technique and quantified via HPLC/PDA analysis. Anthocyanins (92 µM Cyanidin-3-glucoside) proved to exert cytotoxicity on B16-F10 melanoma cells, according to WST-1 assay. Anthocyanins were taken up by melanoma cells, their cellular concentration being quantified by HPLC analysis. In order to easily follow their journey inside the B16-F10 cells, we bound them to a fluorescent compound like Naturstoff Reagent A (NSRA). It is known that anthocyanins express intrinsic fluorescence of rather low intensity. NSRA enhanced the fluorescence of the anthocyanins, with 86.2% of the cells expressing fluorescence after 2h, respectively with 61.5% after 24h as flow cytometry results prove. Therefore this enhanced fluorescence of anthocyanins enabled a better visualization of the anthocyanins inside the melanoma B16-F10 cells, sustaining NSRA to be a useful tool in studies required for distribution and visualization of anthocyanins in melanoma cells.

Poster T4-37

Structural characterization of Fe-incorporated tungsten trioxide used for improving gas sensing

M Osiac[1] **and N Ciotera**[2]

[1] University of Craiova, Faculty of Science, Physics Department, 200595, Romania

[2] University of Craiova, Faculty of Science, Chemistry Department, 200595, Romania

E-mail: m_osiac@yahoo.com

Abstract. In this paper we report the iron doped-tungsten oxide (Fe and WO_3) thin film material to be an attractive candidate for the gas sensing detection. The thin film based on WO_3 with Fe as a dopant is deposited by pulsed laser deposition (PLD) technique. A tungsten oxide and Fe targets were irradiated by a laser with 213nm wavelength. The deposition was carried out in oxygen atmosphere and the temperature of the Silicon substrate was $600^{-}720^{o}$C. The oxygen pressure was varied from 75-250mTorr. The influence of the substrate temperature, gas pressure, amount of Fe on properties of the obtained Iron doped WO_3 was investigated by Atomic Force Microscopy, Raman spectroscopy, Scanning Electron Microscopy coupled Energy Dispersive Spectroscopy and X-ray diffraction.

Poster T4-38

Organic acids as surfactants for magnetic nanoclusters

A Petran, T Radu and R Turcu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: anca.petran@itim-cj.ro

Abstract. Magnetic nanoclusters of magnetite provide interesting properties for biomedical applications if they supply a specific dimension, high magnetization, stability and biocompatibility with the environment for which they are used. Our target was to synthesized new biocompatible magnetic nanoclusters by adjusting the size of clusters using biocompatible organic acids as surfactants by solvothermal method and study their stability in specific pH range and their interaction with the rat blood cells. The obtained clusters provide uniform size below 200 nm, high magnetization between 68-71 emu/g and stable ς potential values for the pH range 6-8, specific for human body. XPS measurement confirm the specific moieties of the organic acids at the surface of magnetic clusters. The results obtained by hemolysis and erythrocyte antioxidant systems show no negative effect after interaction of magnetic clusters with the rat blood cells. **Acknowledgments.** This work was supported by Core project PN-19-35 No.36N/13.02.2019.

Poster T4-39

Plastering Mortar with Organic Natural Polymers Studied By ^{1}H NMR relaxometry

A O Pintea[1], D L Manea[1], C Aciu[1], E Jumate[1] and R Fechete[2]

[1] Technical University of Cluj-Napoca, Faculty of Civil Engineering. 15C Daicoviciu Str., 400020, Cluj-Napoca, Romania

[2] Technical University of Cluj-Napoca, Department of Physics and Chemistry, 25 G. Baritiu Str., 400027, Cluj-Napoca, Romania

E-mail: alexandra.pintea@ccm.utcluj.ro

Abstract. Modern studies onconstruction buildings revealed the use of organic natural polymers as additives for the construction materials. It was demonstrated that by using these additives in composition of plastering mortars the mechanical properties and impermeability was improved. Ten recipes of plastering mortars, with and without organic natural polymers such as casein, rice and egg were studied by 1D ^{1}H NMR relaxometry. For the determination of the T_2 transverse relaxation time distributions, the acquired CPMG decays were analysed using a fast Laplace inversion algorithm. These distributions were obtained for wet and dry plaster mortars which were measured after 28 days from preparation during the hydration of mineralogical components. In almost all cases, the distributions of transverse relaxation times T_2 were characterized by four components associated with hydration water and water inthree types of pores of different dimension. The relaxation ratio ($1/T_2$) of hydration water were correlated with mechanical resistance at elongation and compression and water absorption degree. Among replacement additives the plaster mortar with casein increases the mechanical properties and the formula with egg reduce the water permeability.

Poster T4-40

Electrochemical detection of 8-hydroxydeoxyguanosine with graphene and N-doped graphene modified electrodes

F Pogacean, C Varodi, M Coros, V Mirel, C Socaci, M C Rosu and S Pruneanu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: florina.pogacean@itim-cj.ro

Abstract. 8-Hydroxydeoxyguanosine (8-OHdG) is a typical biomarker of oxidative DNA damage and has attracted much attention in recent years since the level of 8-OHdG in body fluids is typically associated with various diseases. Two graphene-based materials were prepared by exfoliation of graphite rod with pulses of current. The first material (denoted Gr) was exfoliated in a mixture of boric acid and sodium chloride. The second material (denoted NGr) was prepared by exfoliation of the graphite rod in ammonium sulphate and ammonia. Both materials were morphologically and structurally characterized by FTIR, XRD, SEM, and elemental analysis. After preparation, the materials were used for the modification of two glassy carbon electrodes, denoted GC/Gr and GC/NGr, respectively. The performances of each electrode towards 8-OHdG detection were tested in laboratory solutions (pH 6 PBS) containing increasing concentrations of 8-OHdG (10^{-7}–10^{-4} M). Due to its large area and the enhancement of electrons transfer, the GC/Gr modified electrode exhibited excellent electro-catalytic activity and generated higher electrochemical response to 8-OHdG oxidation, in comparison with GC/NGr electrode. **Acknowledgement.** This work was supported by a grant of Romanian Ministry of Research and Innovation, CNCS-UEFISCDI, project number PN-III-P4-ID-PCCF-2016-0006, within PNCDI III.

Poster T4-41

Nanomaterials for water cleaning and purification

M N Pop

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: pop.mircea.n@protonmail.com

Abstract. Water purity with an affordable price is a key factor for sustainable human development in particular and for the environment in general. There is an increasing necessity to clean or purify the water alterated because of natural or human factors. Nanomaterials, due to their increased surface to volume ratio and due to some size- enabled, different than bulk properties, are a promising key solution towards water cleaning and purifification. Yet, employing and fully recovering these materials (often coming in nanometer sized powders) in large- scale applications require certain methodologies and or devices. This paper is a short survey of the developed methods for water purification employing nanomaterials. Emphasis is placed on energy efficient methods for nanomaterials-based water purification.
Acknowledgments. The presented work has been carried out through the Core- Program, developed with the support of the National Innovation and Research Ministry (MCI), project no. PN19 35 02 03

Poster T4-42

Enhanced photocatalytic degradation of Rhodamine B using ZnO:Cu nanoparticles supported on MWCNTs

A Popa, D Toloman, M Stan, M Stefan, S Macavei, C Leostean, L Barbu-Tudoran and O Pana

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: adriana.popa@itim-cj.ro

Abstract. Water pollution is one of the major issues of now days. Over the last few years, various strategies have been developed to solve this problem. Semiconductor-based photocatalysis is one of the most effective approach for water purification. One of the strategies to enhance the photocatalytic activity of semiconductors is to couple them with carbon nanotubes thus ensuring a more efficient separation of photo-induced charge carriers delaying their recombination. Moreover, MWCNTs have the role of photocatalyst supports due to their large specific surface area and good mechanical strength. In the present work, the photocatalytic activity of multi-walled carbon nanotubes (MWCNTs) decorated with different concentrations of ZnO:Cu nanoparticles was tested under visible light irradiation using Rhodamine B as model pollutant (RhB). The formation of composite was confirmed by transmission electron microscopy (TEM), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS) and electron spin resonance (ESR). The band-gap estimation was realized using UV-Vis spectroscopy. By using the ESR coupled with spin trapping technique, the generation of reactive oxygen species resulted by light irradiation of samples was evidenced and their influence on the photocatalytic activity was highlighted.

Poster T4-43

Electrochemical synthesis of nitrogen-doped graphene

S Pruneanu, F Pogacean, M Coros, V Mirel, C Socaci, M C Rosu and C Varodi

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat Street, 400293 Cluj-Napoca, Romania

E-mail: stela.pruneanu@itim-cj.ro

Abstract. Over the last few years, the electrochemical exfoliation of graphite rods for graphene synthesis has attracted increasing attention due to the fact that involves inexpensive apparatus and is generally performed under ambient conditions. In this work, we proposed a novel method which uses short electrical current pulses for the exfoliation of graphite electrodes immersed in aqueous electrolytes. The electrolyte contained various concentrations of ammonia and inorganic salts, and the resulting materials were composed of few-layer and multi-layer graphene, doped with nitrogen. Next, morphological and structural characterization of the prepared materials was performed by TEM, FTIR, XRD and elemental analysis. The influence of the electrolyte composition on the doping process was also investigated. The electrochemical performances of the nitrogen-doped graphene deposited on top of glassy carbon or screen-printed electrodes were also evaluated. **Acknowledgement.** This work was supported by a grant of Romanian Ministry of Research and Innovation, CNCS-UEFISCDI, project number PN-III-P4-ID-PCCF-2016-0006, within PNCDI III.

Poster T4-44

Oxidation of magnetite nanoparticles during their synthesis

M Răcuciu[1] **and S Oancea**[2]

[1] Environmental Sciences and Physics Department, Faculty of Sciences, Lucian Blaga University of Sibiu, Dr. I. Ratiu Street, no. 5-7, 550012, Sibiu, Romania

[2] Agricultural Sciences and Food Engineering Department, Lucian Blaga University of Sibiu, Dr. I. Ratiu Street, no. 7-9, 550012 Sibiu, Romania

E-mail: mihaela.racuciu@ulbsibiu.ro

Abstract. Water colloidal solutions of iron oxide nanoparticles coated with tetramethylammonium hydroxide were synthesized by co-precipitation methods. Dimensional analyses were accomplished by transmission electron microscopy (TEM). The iron oxide nanoparticles structure was investigated by ATR-FTIR and Raman spectroscopic techniques. For nanoparticles sample prepared at higher temperature during synthesis, the Raman spectra revealed that magnetic core of iron oxide nanoparticles is given by the coexistence of magnetite (Fe_3O_4) and maghemite (γ-Fe_2O_3) phases. We suppose that oxidation of magnetite to maghemite have been produced during the preparation protocol of nanoparticles at higher temperature.

Poster T4-45

Au/graphene composites as catalyst for formic acid dehydrogenation

T Radu, O Grad, M Mihet, M Dan, C Berghian-Grosan, G Blanita and D Lazar

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: teodora.radu@itim-cj.ro

Abstract. Gold-graphene composites (Au/rGO) with gold concentration in the range 2.5 wt.% to 10 wt.% were prepared for aqueous formic acid (FA) dehydrogenation. The new composites were examined by various characterization techniques. The Au/rGO composites with Au concentration of 2.5 wt.% present AuNPs of lowest dimension from the analysed samples and proved good catalytic activity for FA decomposition in aqueous solution. The catalytic capacity of obtained samples for the FA decomposition reaction is analysed based on the obtained electronic levels diagram. The small AnNPs reduces the charge carrier transfer distance in Au/rGO composite, which further suppresses the recombination of the electron–hole pairs and therefore enhancement of its catalytic activity is observed. **Acknowledgements.** This work was supported by a grant of the Romanian National Authority for Scientific Research and Innovation, CNCS – UEFISCDI, project number PN-II-RU-TE-2014-4-1326.

Poster T4-46

Thermal treatments of natural zeolite for enhancing their ammonium ions removal capacity from water

D Simedru[1], **A Moldovan**[1], **V Babalau-Fuss**[1], **O Cadar**[1], **B Angyus**[1] **and G Chioreanu**[2]

[1] INCDO-INOE 2000, Subsidiary Research Institute for Analytical Instrumentation Cluj-Napoca, 67 Donath, 400293, Cluj-Napoca, Romania

[2] Zeolites Production S.A., 359 Republicii Street, 505500, Rupea, Romania

E-mail: dorina.simedru@icia.ro

Abstract. In order to obtain a zeolite with enhanced capacity to remove the ammonium ions from water, a natural zeolite from Rupea, Brasov County, Romania was milled and three zeolites with particle size of <5μm; 0,5 – 1,25 mm and 1,25 – 3,0 mm were obtained. The milled zeolites were thermally treated for 6 and, respectively 24 h at different temperatures ranging from 50 to 400 °C. The raw zeolite and the thermally treated zeolites were exposed to waters with high concentration of ammonium ions (~3.2 mg/L NH_4^+) for 1 and, respectively 7 days. The removal capacity was tested using a UV Vis spectrometer. The results showed that the thermally treated zeolite with the particle size of <5μm had the optimum ammonium ions removal capacity. A comparative XRD analysis was performed on raw zeolite with particle size of <5μm and the thermally treated zeolite with the same particle size to identify the structural changes, which may be responsible for enhancing the ammonium ions removal capacity. The XRD patterns identified low variations in the structure of thermally treated zeolites.

Poster T4-47

Reduced graphene oxide as easily available adsorbent for sunset yellow removal

C Socaci, M Coros, S Pruneanu, F Pogacean, M C Rosu, A Turza and L Magerusan

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: crina.socaci@itim-cj.ro

Abstract. Removal of organic azo dyes from waste waters remains an important issue for the scientific community, as they are extensively used in textile, leather, plastic, food processing, cosmetics, paper, printing and dye manufacturing industry. We considered sunset yellow as model synthetic azo dye, known to cause behavioural and hyperactivity issues in children. From the existing removal procedures, adsorption remains the most used because of its simplicity and relatively low cost of application. There are reported sophisticated adsorbent nanocomposites for sunset yellow removal, for example containing polypyrroles and polyanilines, bimetallic Ni-Ag nanoparticles supported on reduced graphene oxide or carbon nanotubes with low to good adsorption capacity. We propose the usage of simple thermally reduced graphene oxide as a very efficient nanosorbent. The structural characterization of the initial nanomaterial in comparison with the sunset yellow adsorbed thermally reduced graphene oxide will be described. The effect of pH, graphene concentration, initial dye concentration, adsorption isotherm models, effect of extraction time and the adsorption kinetics will also be presented. **Acknowledgment**. The financial support for this work was provided by the Ministry of Research and Innovation, program Nucleu, contract no. PN 19 35 02 02.

Poster T4-48

MnO_2/GO – preparation and characterization

M L Soran, O Opriș, I Lung, A Stegarescu, S Guţoiu, S Porav, D Lazăr, S Pintea and O Pană

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat Street, 400293 Cluj-Napoca, Romania

E-mail: loredana.soran@itim-cj.ro

Abstract. Graphene oxide (GO), an important derivative of graphene, has a layered structure with oxygen function groups and a large surface area. Through the attachment of metal-oxides at the surface of GO, the resulted materials can be used in magnetic resonance imaging, magnetic fluid hyperthermia, magnetic separations, biosensors, water decontamination and controlled drug delivery. The aim of this work consists in preparation and characterization of the MnO_2/GO nanocomposites by different techniques (e.g. direct synthesis of MnO_2 from $KMnO_4$ in aqueous solution of GO or attachment of already prepared $MnO_2$to GO). The effect of temperature on the obtained systems was studied in correlation to their structural properties, morphology and magnetic properties. The characterization of samples was performed by XRD, BET, and TEM. Due to their high specific surface these materials can be used in applications like adsorption of different pollutants from waters.

Poster T4-49

Synthesis, characterization and evaluation of photocatalytic activity of some WO_3-MWCNT nanocomposites

M Stan, **A Popa**, **D Toloman**, **M D Lazar**, **T D Silipas and A S Porav**

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: manuela.stan@itim-cj.ro

Abstract. Photocatalysis has emerged as a new method for the treatment of air and water pollutants, including textile azo dyes and phenyl compounds discharged in industrial effluents. Over the last years, carbon nanotube/metal oxide nanoparticle based hybrid structures have become an efficient way to create carbon architectures with new properties and application prospects.In this work, multi-walled carbon nanotube (MWCNT)-tungsten trioxide (WO_3) nanocomposites with different mass ratio of MWCNTs to WO_3 were prepared by precipitation method. The effect of calcination temperature on crystallinity and morphology of WO_3 nanoparticles was studied. XRD, TEM, SEM, FTIR and BET techniques have been employed for the characterization of composite photocatalysts. The prepared nanocomposites were tested for their photocatalytic activity towards the degradation of organic methylene blue (MB) dye.

Poster T4-50

Synthesis and characterization of g-C_3N_4-TiO_2photocatalyst

M Stefan, O Pana, A Popa, D Toloman, C Leostean, M D Lazar, S Macavei and L Barbu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: mstefan@itim-cj.ro

Abstract. In recent years, purification of waste water using natural solar energy to complete degradation of organic and microbial pollutants is a priority task in the general context of energy crisis. Nanocomposites based on two or more components exhibit novel physico-chemical properties concentrated in one single entity with various technological applications. As a classical photocatalyst, TiO_2 is extensively studied material in the field of photocatalysis owing to its abundance, low cost, high photochemical stability and nontoxicity. Graphitic carbon nitride (g-C_3N_4), a polymeric material consisting mainly of carbon and nitrogen, has attracted much attention due to its visible-light activity, nontoxicity and stability. The present work reveals our results regarding preparation and characterization of g-C_3N_4-TiO_2nanocomposites. The preparation conditions of these composites are correlated with the need to obtain electron-hole recombination rates as low as possible, thus increasing the efficiency of the photocatalytic process. Based on the above consideration composite g-C_3N_4-TiO_2nanoparticles were realized by deposition of TiO_2 nanoparticles onto the g-C_3N_4. The method used for preparation of g-C_3N_4 was the thermal decomposition of urea. TiO_2 nanoparticles were obtained by a sol-gel process. The nanocomposites were characterised by X-ray diffraction (XRD), transmission electron microscopy (TEM) and high resolution (HRTEM), UV-Vis spectroscopy, surface area and porosity measurements. Finally, the photocatalytic activity toward the degradation of RhB solution was evaluated.

Poster T4-51

Preparation and characterization of magnetic nanocomposites based on CNT/Fe_3O_4, with sorption properties

A Stegarescu, M L Soran, I Lung, O Opris, S Guţoiu, S Porav, D Lazăr, S Pintea, C Leoştean and O Pană

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: adina.stegarescu@itim-cj.ro

Abstract. Nano-materials used in water treatment are researched widely in the last years. The carbon nanotubes (CNT) are novel inorganic functional nanomaterials with one-dimensional tubular structure. Due to their small dimension, large specific surface area, electrical conductivity and thermal conductivity, CNT possess properties in the fields of battery materials, engineering materials, carbon fibres and biocatalysis materials. In this study, the preparation and characterization (XRD, BET, TEM) of multi-walled carbon nanotubes containing Fe_3O_4 nanoparticles are presented. Due to their large specific surface area and unsaturated surface atomic coordination the CNT/Fe_3O_4 were tested for aqueous solution adsorption of different pollutants like: heavy metal ions, antibiotics, dyes and other organic compounds. After decontamination, the nanocomposite was magnetically separated from the water solution.
Acknowledgments. This work was carried out through the Core Programme, developed with the support of MCI, project no. PN 19 35 02 03 (36N/13.02.2019).

Poster T4-52

Topological superconductivity from magnetic impurities on monolayer NbSe2

D Sticlet and C Morari

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: doru.sticlet@itim-cj.ro

Abstract. It was recently shown experimentally that superconductivity survives in monolayer NbSe2. Moreover, magnetic impurities added on top of superconducting NbSe2 generate localized in-gap bound (Yu-Shiba-Rusinov) states with slow-decaying wave functions. We show that in a chain of such magnetic impurities it is possible due to strong Ising spin-orbit coupling in NbSe2 to stabilize topological phases. We map the topological phases as a function distance between impurities, orientation of the chain on the superconducting substrate, and coupling strength between impurity and substrate. The topological phases are characterized by zero-energy excitations localized at the chain edges (Majorana bound states). Using numerical methods, we analyze several features of these states, which makes them a promising building block for topological quantum computation.

Poster T4-53

Preliminary study on the nano-silver doped TiO_2 synthesized via Pechini method

R C Suciu[1], A Perhaiță[2], A Turza[1] and O Pană[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Institute for Research in Chemistry "Raluca Ripan", Babeș-Bolyai University,400294 Cluj-Napoca, Romania

E-mail: ramona.suciu@itim-cj.ro

Abstract. Ag doped titania nanoparticles were obtained by mixing acetylacetonate-modified titanium(IV) isopropoxide with silver nitrate (the Ag^{+}/Ti^{4+} atomic radio, is respectively 0,5%, 1%, 1.5%. 2% and 2.5%) and the L(+)-ascorbic acid, as reducing agents. Thermal decomposition of the complex in air up to 1400°C shows five decomposition steps, resulting in a total mass loss of 44,75%. Crystalline TiO_2 anatase phase, free from organic residues, forms around 545ºC and the TiO_2 rutile phase close to 800ºC. The band gap value has a blue shift and the PL intensities decreased with an addition of the Ag. The crystalline development in the Ag - TiO2 investigated by X-ray diffraction peak broadening evidence the presence at TiO_2 anatase and Ag nanocrystalline phases. The influence of Ag content on microstructural parameter of TiO_2 anatase was investigated also. **Acknowledgments**. This work was supported by the Romanian Ministry of Education and Research through program, National Core Project PN19 35 02 03.

Poster T4-54

Superconducting qubits for analog quantum simulations of spin lattice models

L Timbolmas[1,2] and L P Zârbo[1]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

[2] Faculty of Physics, Babeș-Bolyai University, 1 Kogalniceanu, 400084 Cluj-Napoca, Romania

E-mail: larisa.timbolmas@itim-cj.ro

Abstract. We introduce a quantum simulation platform for simulating effective spin models using solid state electrical circuits containing Josephson junctions. Our quantum simulator model contains two arrays of loops divided by Josephson junctions in which the fluxons can tunnel between neighboring sites. We obtained the circuit Hamiltonian studied theoretically the dynamics of the fluxons through the circuit. We calculated the energy levels of the coupled qubit system and performed the mapping between the circuit variables and the spin lattice models, proving that our theoretical superconducting circuit configuration could be used to perform analog quantum simulations of these models.

Poster T4-55

MWCNT decorated with ZnO nanoparticles embedded in PVDF membrane for water treatment

D Toloman, A Popa, M Stefan, M Stan, S Macavei, C Leostean, L Barbu-Tudoran and O Pana

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: dana.toloman@itim-cj.ro

Abstract. Photocatalysis technology is an effective and green method for the removal of organic pollutants from water. The catalyst loss in separation from suspension system represents an important drawback of photocatalytic technology. This issue could be solved by immobilization of catalyst on porous materials like activated carbon and membranes. Membrane filtration technology can efficiently separate suspended solids, bacteria and macromolecule solutes. By combining photocatalysis and membrane filtration technology the efficiency of pollutants treatment can be enhanced due to a series of synergistic effects. Based on the above considerations, in the present study we have synthesized and characterized multiwalled carbon nanotubes (MWCNTs) decorated with zinc oxide (ZnO) nanoparticle and blended in polyvinylidene fluoride (PVDF) membrane by casting from solution. Membranes containing ZnO/MWCNTs nanocomposites were further characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), UV-Vis and XPS spectroscopy. Next, the effect of the embedded nanocomposites on the morphology, porosity and photocatalytic performances of PVDF blended membranes under UV irradiation was studied. Rhodamine B (RhB) dye solution was used to evaluate the photocatalytic response of both standalone catalyst and composite membrane. The photocatalytic mechanism was elucidated based on the identification of radical species involved and by considering the energy bands alignment between ZnO and MWCNT and the membrane porosity. The presence of radical species at the solid–liquid interface was evidenced using ESR experiments coupled with the spin-trapping technique.

Poster T4-56

Challenges in metallic nanoparticles synthesis and prospective applications

M A Ujica[1], A Mocanu[1], D A Chira[1] and M Tomoaia-Cotisel[1,2]

[1] Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Research Center of Physical Chemistry, 11 Arany Janos str., RO-400028, Cluj-Napoca, Romania

[2] Academy of Romanian Scientists, 54 Splaiul Independentei, RO-050094, Bucharest, Romania

E-mail: ujica_madalina@yahoo.com

Abstract. This study provides a comprehensive view on the synthesis of silver nanoparticles (AgNPs) and gold nanoparticles (AuNPs) and on their biological and medical applications. The focus is on the effective and safe synthesis of these metallic nanoparticles, while trying to understand the current scenario in the debates on the toxicity concerns on these nanoparticles. Simultaneously, this study explores their various prospective applications. **Acknowledgement.** Authors thank to UEFISCDI for financial support through the grant no. 83.

Poster T4-57

Photocatalytic self-cleaning ability of Ag/TiO_2-coated flax fabrics

A Urda[1], D Cosma[1], R C Suciu[1], C Socaci[1], M Coros[1], S Pruneanu[1], F Pogacean[1], A Turza[1], M C Rosu[1], L Chirila[2], A O Mateescu[3] and D Timpu[4]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania
[2] National Research & Development Institute for Textiles and Leather, 16 Lucretiu Patrascanu Street, 030508, sector 3, Bucharest, Romania
[3] "Horia Hulubei" National Institute for Research and Development in Physics and Nuclear Engineering, 30 Reactorului Street, 077125, Magurele, Romania
[4] "Petru Poni" Institute of Macromolecular Chemistry, 41A Grigore Ghica Voda Alley, 700487 Iasi, Romania

E-mail: alexandra.urda@itim-cj.ro

Abstract. Ag-TiO_2 nanoparticles were prepared by sol-gel methodand characterized by XRD, FTIR and UV-VIS spectroscopy. Flax fabrics were treated with Ag-TiO_2 nanoparticles and then stained by tea of forest fruits. The photocatalytic self-cleaning ability of Ag/TiO_2-coated flax fabrics was investigated by the discoloration of tea stains under UV/visible light irradiation. The colour parameters (L, a, b) according to CIELAB system were measured and the colorimetric analysis was performed. The experimental results showed that the photocatalytic self-cleaning ability of the Ag/TiO_2-coated flax fabrics was superior to the flax alone. **Acknowledgments.** This work was supported by a grant of Romanian Ministry of Research and Innovation, CCCDI – UEFISCDI, Project number PN-III-P1-1.2-PCCDI-2017 0743/44PCCDI/2018, within PNCD III.

Poster T4-58

Screen-printed electrodes modified with graphene for the detection of 8-OHdG in biological fluids

C Varodi, F Pogacean, V Mirel and S Pruneanu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat Street, 400293 Cluj-Napoca, Romania

E-mail: codruta.varodi@itim-cj.ro

Abstract. Reactive oxygen species (ROS) are constantly generated during metabolic processes. DNA can be damaged by oxidative processes which could give rise to carcinogenesis and aging. Guanine, one of DNA bases, is the most susceptible to oxidative damage due to its low oxidation potential, leading to the formation of 8-hydroxy-2'-deoxyguanosine (8-OHdG). The concentration of 8-OHdG into urine may reflect the extent of total body DNA oxidative damage. In this work, we employed screen-printed electrodes modified with graphene for the electrochemical detection of 8-OHdG both in laboratory solutions and in biological fluids (urine and saliva). The performances of such electrodes in terms of linear range and limit of detection were compared with those of unmodified screen-printed electrodes. **Acknowledgement.** This work was supported by a grant of Romanian Ministry of Research and Innovation, CNCS-UEFISCDI, project number PN-III-P4-ID-PCCF-2016-0006, within PNCDI III.

Poster T4-59

The influence of the solvent on the microwave obtaining of platinum nanoparticles on graphene oxide

F Vasut, A Oubraham, A Soare, A Marinoiu, M Dragan, C Sandru and D Ebrasu-Ion

National Research and Development Institute for Cryogenic and isotopic Technologies - ICSI Rm. Valcea, Rm. Valcea

E-mail: felicia.vasut@icsi.ro

Abstract. ICSI Ramnicu Valcea developed a detritiation process of used heavy water from CANDU reactors. Separation of hydrogen isotopes is important for nuclear technology in order to recover tritium for fusion industry. The process takes place in heterogenous phase and is assisted by a catalyst. The catalyst contains commercial platinum on carbon and polytetrafluoroethylene. Graphene and graphene oxides have been investigated as support material for noble metals due to their excellent physical and chemical properties. The high specific surface, their thermal and chemical stability, high mechanical strength makes graphene a potential component for the development of new catalysts that could be used in the process of isotopic exchange. Also, the microwave irradiation techniques were proved to be a rapid and high effective strategy for the preparation of graphene-based materials. The paper presents a new method for obtaining Pt on graphene oxide in the presence of different solvents like reducing agents (ethylene glycol, acetone and ethanol) in order to obtain small crystals and good dispersion of the metal on the graphene oxide surface. This work presents the results of BET, SEM, TGA and XRD analysis for the in-house prepared powder Pt/graphene oxide to reveal the microstructural differences between the materials.

Poster T4-60

Electrical properties of supported graphene-based materials

L M Veca[1], C Socaci[2], F Nastase[1], A Istrate[1], E Pavelescu[1] and A Dinescu[1]

[1] National Institute for Research and Development in Microtechnologies, 126A Erou Iancu Nicolae, 077190, Bucharest, Romania;

[2] National Institute of Research and Development for Isotopic and Molecular Technologies, Donat 67-103, 400293 Cluj-Napoca, Romania

E-mail: monica.veca@imt.ro

Abstract. Graphene-based materials are showing increased attention in the field of nanoscale optoelectronic devices (photovoltaics, light emitting diodes, photodetectors) owing to their high mobility, mechanical strength, wavelength-independent absorption across a wide energy range, and ease of processability. Among all, transport properties are critical for the optoelectronic applications and very sensitive to the graphene/substrate interaction, defects density, and thickness (number of stacked graphene layers). In this context, we carried out a systematic study of the transport properties in different graphene-based materials such as single layer graphene (SLG), multi-layer graphene (2L,3L,4L), as well as graphene oxide with various degrees of oxidation and chemical doping with heteroatoms. While graphene of commercial provenience grown by chemical vapour deposition on copper foil has transferred layer-by-layer on the n+-Si/SiO_2 (300 nm) substrates using electrochemical delamination method, graphene oxide and its derivatives were deposited from suspensions of different concentrations. The active and metallic contact areas were defined through conventional e-beam lithography, which allows a precise control over the structure and placement of metallic contacts. All devices have been tested in a wide range of source-drain and gate biasing conditions to assess their technological viability as the photodetector's conduction channel.

Micro-symposium:

New Trends in Alternative Energies

Oral M1

Innovative energy service solutions for buildings integration into the energy market

A Ceclan, D Stet, L Czumbil, M Cretu and D D Micu

Technical University of Cluj-Napoca, Electrical Engineering Faculty, 400027, Cluj-Napoca, Romania

E-mail: andrei.ceclan@ethm.utcluj.ro

Abstract. Technical University of Cluj-Napoca, through a series of Horizon 2020 ongoing or implemented projects launched a holistic approach for the buildings integration into the energy market. Thus, TUCN implemented and tested, using its own public aggregated or individual buildings, a series of innovative technologies - RES, CHP, energy monitoring system - and energy services as Demand Response in Blocks of Buildings. In this paper, the successfully implemented DR BoB project is presented, with highlights on the achieved results and future steps.

Oral M2

Integrated computing unit for autonomous solar tracker with concentrated power

S Gergely, A Bot, V Rednic, R Gutt, E Bruj, R Pop, R Gavrea, S Pogacian and N Aldea

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat st., 400293 Cluj-Napoca, Romania

E-mail: stefan.gergely@itim-cj.ro

Abstract. The usage of solar concentrators to produce energy, requires a system of tracking the sun's trajectory throughout the day. Accurate moving of the tracking system requires precision positioning of the concentrated energy in a single or multiple focal points. The calendar variation of the solar trajectory implies a high-precision computing system, able to perform real-time orbital computations. Thus, calculating solar coordinates using the method of astronomical ephemeris with GPS synchronization implies significant calculation power. The calculations are performed by optimizing the resolution at the level of under 1/100 angular degrees, therefore it was necessary to use the double precision format. The obtained solar coordinates represent the positioning reference for controlling the drive motors in the azimuthal direction respectively on the elevation. The system is designed to ensure the self-monitoring of the tracking system and does not require an external computer. The computing system must meet the necessary criteria for industrial equipment, where most PC hardware does not meet the operating conditions below 0°C. The hardware design of the computing system was intended to optimize self power consumption while also providing the full range of required interfaces. Also, an essential criterion was to get a low final price for the entire designed computing system.

Oral M3

Analysis of measuring wind resource on solt field in Yeonggwang-Gun

Hyenjun Choi, Yeonhee Kim, Jinhoon Park and Mansoo Choi

Green Energy Institute (GEI), 177 Samhyangcheon-ro, Mokpo-si, 5856, Republic of Korea

E-mail: hjchoi@gei.re.kr

Abstract. In order to construct a wind farm suitable for the region, it is necessary to select type of a wind turbine and design a wind farm. To do this, a precise survey of the wind speed and direction in the candidate area should be preceded based on the actual wind data of the candidate area. For analysis of quality of the wind speed and direction on the candidate area, data measured at the hub height of the wind turbine to be installed in the candidate area are needed. The data are at least one year of atmospheric precipitation data. Based on the data, the monthly, seasonal and annual wind speed and direction of the candidate area are analyzed. This study is the analysis of measuring wind resource on solt field in Yeonggwang-Gun, Korea. The data are measured at the wind mast where height is 83m. Based on the actual wind speed and direction data, the quality of wind speed and direction of solt field in Yeonggwang-Gun are analyzed by WindPRO about monthly, seasonal, and annual wind data.

Oral M4

Environmental-friendly methods to recycle silicon wafers fron end-of-life photovoltaic modules

Jongsung Park, Nochang Park, Changheon Kim and Sukho Lee

Green Energy Institute (GEI), 177 Samhyangcheon-ro, Mokpo-si, 5856, Republic of Korea

E-mail: jspark@gei.re.kr

Abstract. In this abstract, we present our methods to recycle silicon (Si) wafers from end-of-life (EoL) photovoltaic (PV) modules. In order to separate each layer of solar modules, we annealed the solar modules in a furnace with a specially designed fixture. We developed three different technologies to remove the impurities of wafer surface. These include: (i) Two steps chemical etching method, (ii) combination of chemical etching and mechanical grinding method and (iii) etching paste method shown in Figure 1. The method (i) consists of ARC and Al etching using H_3PO_4 and both Ag electrodes and emitter etching using mixed HF and HNO_3 solution. The second method includes Ag electrode etching using HNO_3, emitter removing using mechanical grinder, and Al etching using KOH. The third method is composed of Ag and Al etching using HNO_3 and KOH, respectably, and ARC and emitter removing via etching paste containing H_3PO_4.

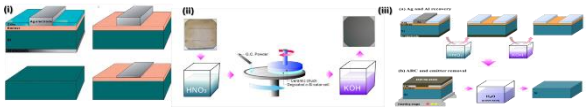

Fig 1 The method to remove the impurities of wafer surface (i) 2 steps chemical etching methods, (ii)combination of chemical etching and mechanical grinding method, and (iii)

Oral M5

Digitization and challenges of energy industry

O Raita

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat st., 400293 Cluj-Napoca, Romania

E-mail: oana.raita@itim-cj.ro

Abstract. Digital technologies are everywhere, affecting how we live, work, travel and even play. Digitization contributes to improving the safety, productivity, accessibility and sustainability of energy systems around the world. But, it also raises new security and confidentiality risks, while disturbing markets, businesses and workers. By learning from other industry transformation cycles, the digital transformation of energy will go through the same disruptive journey, which makes the status quo no longer an option. Digital energy transformation will help system operators make rational decisions and at the same time gain benefits and value-added services every day. Digital technologies are designed to make the European energy system more connected, smarter, more efficient, safer and more sustainable. Data collection and exchange grow exponentially, creating digital threats but also valuable opportunities. In this context, which is evolving rapidly, the European energy industry has both the challenge and the opportunity to reinvent itself. I will focus in my presentation on how the companies from TREC Cluster use digitalization in their processes and which are the challenges of it they can address.

Oral M6

Two-stage heat recovery system from Stirling engine flue gas

V Rednic, A Bot, R Gutt, S Gergely, E Bruj, R Pop, R Gavrea, S Pogacian and N Aldea

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: vasile.rednic@itim-cj.ro

Abstract. The flue gas resulting from Stirling engine combustion chamber still contains an important part of thermal energy. Our propose was to develop a two-stage heat recovery system, capable of extracting most of the wasted heat. In the first stage a counterflow heat exchanger is used. The thermal energy recovered in this stage is used to preheat a thermal agent. In the second stage the wasted heat is converted in electrical power through thermoelectric devices and another part is recovered as thermal energy through the cooling system of thermoelectric devices as domestic hot water. The numerical simulation used in this research are performed in ANSYS software, using Fluent to simulate fluids flow, temperature distributions and both energy loss and energy transferred through the heat exchangers. **Acknowledgment**: This paper was financially supported from the MCI, Nucleu-Program, project nr.PN 19 35 01 01.

Oral M7

Rectifier antenna efficiency measurements on harvesting electromagnetic field

E Surducan, V Surducan, R Gutt and C Neamtu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat st., 400293 Cluj-Napoca, Romania

E-mail: emanoil.surducan@itim-cj.ro

Abstract. We have manufactured a rectifier antenna (rectenna) composed by an antenna and a rectifier circuit, operating in a specific electromagnetic frequencies range. In order to optimise rectenna efficiency we were interested in three answers for the following questions: (i) how rectenna efficiency depends on power density variation; (ii) how rectenna efficiency is affected by load and what is the best adapted load value; (iii) how the efficiency of the rectenna system (composed by many individual rectena) depends on the rectenna number N on system, for the same electromagnetic power density. Here we present the answers based on the rectenna efficiency measurements.

Oral M8

Experimental technology for improving lead-acid battery resistance to mechanical vibration

C Tudoran and C Neamtu

National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat st., 400293 Cluj-Napoca, Romania

E-mail: ctudoran@itim-cj.ro

Abstract. In this study we briefly present an innovative technology of cold plasma activation and treatment of lead-acid battery electrode grids, developed by our team with the aim to improve the grid's electrical conduction properties and resistance to mechanical vibrations. The technology is based on the use of the effects of atmospheric pressure cold plasma to initiate controlled corrosion and activation processes of lead-acid battery electrode grid surfaces in order to increase the formation of improved lead dioxide conductive layers. The action of the plasma discharge on the metal surface of the grid also increase the roughness at a microscopic scale, the active mass paste adhering better to this surface. As a result of better adherence of the active mass on the surface of the metallic grids, we obtain an increased resilience of the entire battery to the effects of mechanical vibrations - the detachment of the active mass cells from the grid-electrodes is one of the main effects that prematurely ruins a lead-acid battery. As the lead-acid battery manufacturing industry is trying to find new solutions for producing durable batteries intended to be used in harsh conditions, the technology we developed will successfully contribute to solving the problem mentioned above.

Oral M9

A study on independent micro-grid algorithm using complex distributed resources

Woohyoung Lee, Hyunju Oh, Seohyun Yeo and Ko Jaeha

Green Energy Institute (GEI), 177 Samhyangcheon-ro, Mokpo-si, 5856, Republic of Korea

E-mail: whlee@gei.re.kr

Abstract. Recently, a lot of renewable energy has been supplied and diffused in accordance with the Koreans government's policy to spread new and renewable energy. Studies on the Micro-grid, linked to the various distributed resources and ESS (Energy Storage System), are actively conducted. We established a Micro-grid system containing PV, ESS and CHP (Combined Heat and Power) at five factories in the Industrial complex, and conducted tests in a mode for independent operation of the individual factories and operation mode linked the various factories. In this paper, the algorithm independent operation is explained.

Author Index

D

K

L

M

N

O

P

U

V

W

X

Y

Z