13th International Conference

PROCESSES IN ISOTOPES AND MOLECULES

Cluj-Napoca 2021

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Welcome at PIM 2021

It is a pleasure of the National Institute for Research and Development of Isotopic and Molecular Technologies to host the 13th 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 2021 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: *Celebrating half century of Magnetic Resonance in Romania* is scheduled in the last day, in parallel with the regular scientific sessions.

Topics:

T1 – Stable Isotopes, Labeled Compounds and Analytical Techniques

T2 – Molecules, Biomolecules and Green Technologies

T3 – Energy Efficiency and High-Tech Engineering

T4 – Nanostructured Materials - Nanocomposites and Hybrid Materials

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

ABSTRACTS

Plenary Pl-1

High Added Value Molecules in food for better nutrition

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Abstract. Food is a very complex system of different substances with different positive or negative impact in human nutrition. Those with positive impact, nutrients, could be proteins, lipids, carbohydrates, vitamins, minerals, dietary fiber, polyphenols, antioxidants, so on, with specific, but important role in the well-functioning of the organism. Some of them are complementing each other or leads to synergetic effects in their availability to the organism. They may contribute to consumers' health and well-being when incorporated into food matrices in different proportions through increase of essential nutrients and bio-active compounds, High Added Value Molecules (HAVM), in the diet. HAVM include chemo-protective compounds such as dietary fibers, biopeptides, amino acids, microelements and vitamins, phyto-chemicals, pro and prebiotics, etc. These compounds, in very small quantities, have an essential role in protecting organism against harmful environmental factors. The growing awareness that food should not provide only a source of energy, but have also a significant positive effect on human health and lifestyle diseases, puts also emphasis on bioactive components coming from agri-food sources or even arising from by-products as a new food raw material source, within Circular Economy concept.

Plenary Pl-2

Nanostructured materials for sensing applications

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Abstract. Advanced two-dimensional materials and artificial intelligence for chemical and biological sensing devices will be described. We will review results in electrochemical sensing methods, as well se the fabrication and uses of two-dimensional materials such as graphene as well as transition metal dichalcogenides. I will also outline an intelligent system for the detection of viruses, in the context of Risk Prevention, developing solutions to counter and contain the effects of any future pandemic. It is a micro-platform equipped with an innovative technology for real-time detection of the presence of viruses in human breath and aerosol, such as human coronavirus (using for experimentation low pathogenicity strains such as 229E - Alphacoronavirus - or OC43, Betacoronavirus). Such an achievement will be an unprecedented breakthrough, as no technology capable of such monitoring is currently available. The proposed sensing system will be applicable to both face masks (indoor and outdoor use) and air conditioning systems. The proposed sensing will be bound to membranes of conductive nanomaterials, on which selective antibodies to the target viruses have been immobilized, and then deposited on screen printed electrodes (SPE). The determination of the presence of the virus in the aerosol will take place in real time in a label-free manner, i.e. without the addition of reagents, through the measurement of the electrical pulse or the variation of the current of current (at potential applied at the ends of the membrane) following the formation of the virus/antibody-membrane complex. Signal processing will also rely on artificial intelligence (AI) paradigms to mitigate uncertainty related to changes in environmental and operational conditions.

Plenary Pl-3

Recent advances in compound specific Stable Isotope Ratio Analysis for natural products authentication

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Abstract.

Stable isotope ratio analysis of bio-elements (hydrogen, carbon, nitrogen, oxygen and sulphur) has been used to check food authenticity and traceability for more than 30 years for a wide variety of food commodities and in the last years also for some pharmaceutical and cosmetic products. The use of stable isotope analysis for products authentication purposes is based on the fact that several processes and reactions (biological, biochemical, physical, chemical etc.) fractionate individual isotopes of an element and consequently generate 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, sugars, amino acids) can be used to determine authenticity and traceability of a product. In particular it can be used to detect if the origin of an ingredient is synthetic, biotechnological or natural and can be used to verify the origin of agri-food products and to characterise natural products and compounds used in the pharmaceutical and cosmetic sectors. The isotopic fingerprint represents an effective tool for the authenticity assessment of economically (and not only) important natural pharmaceutical, cosmetic and food products.

Plenary Pl-4

Electrophoresis-thermal lens based method for separation and online detection of nanoparticles and biomolecules in microdevices

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Abstract. Thermal lens spectrophotometry coupled with gel electrophoresis represents a powerful tool for separation and detection of a wide range of biomaterials. Still, it often requires prolonged procedure between detection and separation, which can degrade the quality of obtained results. We demonstrated an innovative miniaturized gel electrophoresis chip coupled with thermal lens detection to monitor DNA surface coverage. This system has a reduced buffer and gel volumes of 75 µL and 100 µL, respectively. In our design, 13 nm AuNPs were biofunctionalized with DNA molecules as well as with a mixed self-assembled monolayer of thiol terminated ssDNA and of a thiolate terminated with an oligo ethylene glycol moiety referred to as TOEG6. To validate the functionality of our system, we monitored the electrophoretic mobility of conjugates and DNA-AuNPs with different molar ratios to investigate the degree of DNA surface coverage within four minutes. To further demonstrate the feasibility and practicability of the system, we evaluated the separation capability on the synthesized Fe_3O_4–Au core-shell nanoparticles. The findings showed that the two populations of Fe_3O_4–Au core-shell and Fe_3O_4 particles were effectively separated in less than five minutes, demonstrating a rapid assessment of the nanomaterial quality.

Plenary Pl-5

How ^{13}C isotopic labelling has helped solid-state NMR reveal the molecular architecture of wood

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Abstract. Wood is a complex organic nanocomposite material with desirable properties for the bio-energy, timber and pulping and paper industries. Wood is mainly analysed by sequential degradation to study the different constituents present within the cell walls. However, by breaking down the wood structure any information about its molecular architecture is lost. Solid-state NMR is a powerful technique that is ideal for in-situ structural analysis of wood however, due to the low natural abundance of ^{13}C, the majority of previous solid-state NMR studies of plant material have been restricted to 1D experiments. The ability to grow plants, including wood, in a fully ^{13}C labelled CO_2 environment enables much more sophisticated 2D NMR experiments to be undertaken in accessible timeframes. The combination of several 2D NMR experiments available provides insight into both differences in molecular conformations as well as the relative distances between the key components within the secondary cell wall of the wood. Furthermore, the changes at the molecular level that occur on drying and on rehydration can also be determined.

Plenary Pl-6

Neutron Activation Method applied to environmental, geological, nanomaterial and heritage material samples

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Abstract. Neutron Activation Analysis (NAA) is well known as a sensitive analytical technique useful for performing both qualitative and quantitative multi-element analysis of major, minor, and trace elements in samples from almost every possible field of scientific or technical interest. For many elements and applications, NAA offers sensitivities that are superior to those achievable by other methods. In addition, because of its accuracy and reliability, NAA is generally recognized as the "referee method" of choice when new procedures are being developed or when other methods yield results that do not agree. Some applications of NAA in environmental, geological and heritage studies, as well as in material science are presented. The advantages and drawbacks of NAA as complementary method of investigation of the solid samples are also provided.

Plenary Pl-7

Nanostructured porous materials for environmental catalysis

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Abstract. The nineties constitute a turning point in the development of nanostructured materials with controlled porosity thanks to the successive discoveries of mesostructuration and macrostructuration routes. Derivated hierarchical porous objects are able to cumulate properties related to the different dimensions afforded. Whereas catalytic transformation is strictly depending on the nanoscale, transport properties of species are depending of higher porosity scales (i.e. macroporosity). Dimension, morpholigical properties of porous networks at the nano- and macro- scales of the support must be well balanced in order to maximise reactant transport within the catalyst grain. At the light of these considerations, my work is dedicated to the application of different approaches and strategies to design structured oxides with the help of structuring agents of which the size can be modified from the nanometer scale to the micrometer scale. Hence, for the last ten years, I have developed and optimized porous and surface properties of different classes of materials in order to improve their catalytic performances toward environmental processes (automotive depollution, water depollution…), while trying to take into account phenomena involved in their global efficiency. Numerous applications can be valorized from the use of these multiporous objects exhibiting complex architectures.

Plenary Pl-8

Dark Matter discovery through a 350 m cryogenic isotopic distillation column by the Aria Project: status, results and beyond

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Abstract. The search for Dark Matter is one of the most fascinating themes of modern physics and astrophysics, but also one of the most difficult to study. The innovative Aria project is part of this context and a fundamental pillar of the Argon Dark Matter search program, led by the Global Argon Dark Matter Collaboration. The plant consists of a 350m cryogenic isotopic distillation column, which is longer than the Eiffel tower and made up of about 3000 distillation stages. It is the tallest distillation column ever built and is currently being installed in a mine shaft at CarboSulcis S.p.A. in Italy. The purpose of the column is to purify the Underground Argon (UAr which is rich in ^{40}Ar) that has been extracted from underground sources. Following extraction, this purified UAr will be used as liquid scintillator for the DarkSide-20k detector. In addition, Aria intends to separate other rare and stable isotopes such as ^{15}N, ^{18}O, and ^{13}C, which have applications in other fields such as medical diagnostics, nuclear medicine and many more. In this talk, we will discuss the Aria plant, the status of its construction, the latest results, and its future perspectives in terms of research and commercial usages.

Plenary Pl-9

High-Field Solid-State Nuclear Magnetic Resonance on Low Natural Abundance Isotopes

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Abstract. Nuclear Magnetic Resonance experiments on low natural abundance isotopes, like ^{43}Ca, ^{25}Mg, or ^{17}O, are often used for structural characterization of advanced materials in order to find ways to improve their properties. For example, oxygen atoms line up and form the inner walls of zeolites, and they are critical in hydrogen bonding of biological molecules and pharmaceutically active ingredients. Calcium is critical for the characterization of octacalcium phosphate and its hybrid derivatives for structural characterization of bone and biomaterials. Magnesium is often used for structural characterization of materials with cementitious properties. These are quadrupolar nuclei with low NMR sensitivity, and therefore high magnetic field is crucial to enhance the resolution and the sensitivity. In this talk I will present recent results obtained at the High-Field Solid-State NMR National Facility in UK on such nuclei and I will describe the sensitivity enhancement techniques we use, including saturation of the satellite transitions, and indirect detection via ^{1}H where a small amount of sample is subjected to very fast rotation about the so-called magic angle. I will also present resolution enhancement techniques like double angle rotation, and two-dimensional experiments where the signal of the satellite transitions or the multiple quantum transitions is used to cancel part of central transition broadening.

Plenary Pl-10

Thermal history of planetesimals: what can we learn from meteorites and fluid mechanics experiments

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Abstract. Radioactive decay of unstable isotopes is one of the main heat sources in the early stages of planetary formation. Laboratory studies characterized by Rayleigh and Prandtl numbers in the range relevant for planetary bodies had remained beyond the ability of the experimental approach until the development of a new technique based on microwave heating. Using this technique, we performed a series of experiments focused on the thermal evolution of an internally heated viscous fluid cooled from above. We established a steady-state scaling law relying the internal temperature variation to the Rayleigh number and we showed that this scaling law remains valid during the transitory regime provided both internal heating and secular evolution of the temperature are taken into account. The result is a parameterized model describing the average internal temperature of the fluid as a function of time in terms of experimental conditions and fluid properties. Data from meteorites (melting temperatures, ages, cooling rates) are then used to constrain their parent bodies' thermal history.

Plenary Pl-11

The ELI-ALPS user facility: ultrafast, broadband light sources for diverse applications

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Abstract. The Extreme Light Infrastructure – Attosecond Light Pulse Source (ELI-ALPS) facility is a unique research infrastructure with light sources spanning between the terahertz (THz) and extreme ultraviolet (XUV) wavelength ranges with ultrashort (from few picosecond to attosecond) duration and broad bandwidth. With the recent establishment of the Extreme Light Infrastructure European Research Infrastructure Consortium (ELI ERIC) the doors of the ELI pillars are open for researchers, industry and countries to gain access to the world's largest collection of powerful and ultra-fast lasers for applications in a wide range of scientific disciplines. In my presentation I will present the available infrastructure at ELI-ALPS, describing their parameters, showing examples of commissioning user experiments, and highlighting planned upgrades broadening the capabilities of light and other secondary radiation sources at our institute.

Plenary Pl-12

Protein formulation through automated screening of pH and buffer conditions using the Robotein® high throughput facility

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Abstract. Among various factors, the direct environment (e. g. pH, buffer components, salts, additives, etc…) is known to have a crucial effect on both the stability and activity of proteins. In particular, proper buffer and pH conditions can improve their stability and function significantly during purification, storage and handling, which is highly relevant for both academic and industrial applications. It can also promote data reproducibility, support the interpretation of experimental results and, finally, contribute to our general understanding of the biophysical properties of proteins.In this study, we have developed a high throughput screen of 158 different buffers/pH conditions in which we evaluated: i) the protein stability, using differential scanning fluorimetry and ii) the protein function, using either enzymatic assays or binding activity measurements, both in an automated manner. The modular setup of the screen allows for easy implementation of other characterization methods and parameters, as well as additional test conditions. The buffer/pH screen was validated with five different proteins used as models, i.e. two active-site serine β-lactamases, two metallo-β-lactamases (one of which is only active as a tetramer) and a single-domain dromedary antibody fragment (V_HH or nanobody). The formulation screen allowed automated and fast determination of optimum buffer and pH profiles for the tested proteins. Besides the determination of the optimum buffer and pH, the collection of pH profiles of many different proteins may also allow to delineate general concepts to understand and predict the relationship between pH and proteins.

Plenary Pl-13

Authenticity and traceability of food: new perspectives and challenges

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Abstract. The development and application of analytical tools to verify the geographical, production and species origin of food products are important topics in food science. Stable isotopic fingerprinting has proven to be a reliable approach for characterizing food commodities according to their origin and authenticity. It also makes it possible to record various environmental, chemical and biological processes linked to food origin and production techniques. The use of isotopes can be even more effective when combined with elemental composition.

This presentation will discuss the principles of isotope analysis, outline the requirements and specific features of the technique in the area of food authentication and traceability, and survey applications of isotope analysis in different types of food production. Specifically, it will focus on recent progress in (i) food adulteration (aroma profiling, fruit juices, honey); (ii) verification of the geographic origin of food (olive oil, fruits and vegetables, milk and dairy products); and (iii) authenticity of organic food (wheat, wine). The classical approaches investigating bulk hydrogen, carbon, nitrogen, oxygen and sulfur isotopes and strategies including compound-specific analysis will also be reviewed. The presentation will also stress the need for standardized protocols to allow comparisons with existing data. Finally, the limitations and future research directions of isotope analysis in food authenticity and traceability will be presented. All examples will be put in the context of relevant projects and infrastructure focusing on industrial needs, including ISO-FOOD, METROFOOD-RI, FNS-Cloud and FoodTraNet.

Plenary Pl-14

Extreme Ultraviolet to soft-X-ray Photonic Integrated Circuits

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Abstract. Today's integrated photonic circuits are based on semiconductor platforms over which several devices can be integrated to provide complex optoelectronic functionalities at very high processing speeds. Absorption restricts operational photon energies below the material band gap, i.e. in the infrared-visible region. Despite the large number of potential applications and the continuous improvement of wide-gap materials, the extension of standard integrated photonics beyond the near ultraviolet appears a formidable task. This extension becomes just unrealistic in the spectral region from the extreme ultraviolet to the soft-X-rays (EUV-SXR) that is severely absorbed by matter. However, such extension is very attractive since EUV-SXR technologies provide sensitive analytical probes on the tiniest spatial (nanometers) and temporal (attoseconds) scales. In this talk, a novel route towards the realization of EUV-SXR photonic integrated circuits will be presented and some applications that may be enabled by this technology will be discussed.

Plenary Pl-15

Studies on biomolecules modeling UV induced DNA/Protein cross-linking

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Abstract. The interaction between nucleic acids and proteins regulates various biochemical processes; DNA replication, protein synthesis, or cellular replication are few cases. Considerable attention has been paid to the interactions of RNA and micro-RNA with proteins of the cell nucleus, and therefore DNA, with protein partners. The inherent complexity of DNA/protein adducts makes the experimental and computational interpretation of smaller model systems extremely useful, if not mandatory. In this respect, 5BenzylUracil (5BU) and 6BenzylUracil (6BU) are very promising candidates. They undergo intramolecular photocyclization when irradiated with UV light (250–260 nm), which makes them potential models for UV-induced cross-linking reactions. Our recent study of the ultrafast dynamics of 5BU, from sub-ps to ns, upon 266 nm excitation aimed to distinguish the ultrafast dynamics of the initial molecule from that of the photocyclized product. We found a new fluorescence band in the deep UV (310 nm) appearing on ultrashort time scales. This is fundamental to determine the scenario of 5BU photo-dynamics. Our simulations in 5BU indicated two main decay routes of excited 5BU: a non-radiative decay to the ground state, and a photochemical pathway, involving the cyclisation of Uracil and Benzene moieties and the final formation of the photocyclized product, called 5,6BU. In the next step to our investigations, we'll perform valence photoemission (PES) and photoelectron-photoion coincidence (PEPICO) measurements on these molecules.

Plenary Pl-16

Particle clustering and structuring phenomena in ferrofluids: advanced investigations, controlled processes and applications

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Abstract.

An overview on recent progress in synthesis and advanced characterization of engineering and bio-ferrofluids, as well as ferrofluid-based magnetorheological (MR) fluids will be presented. Magnetic dipole-dipole interactions between particles in the composition of magnetically controllable fluids (MCFs) are monitored by the values of the interaction parameter λ spanning from $\lambda<1$ for true ferrofluids to $\lambda\sim10^8$ for MR fluids, the bio-ferrofluids (actually multi-core nanosystems) being characterized by intermediate values. By well-established synthesis procedures the magnetic and flow properties, in particular the desired value of the interaction parameter of a MCF is tailored to the requirements of each application, such as leakage-free rotating seals or semiactive magnetorheological devices. Recent results of advanced characterization (among others, electron and optical microscopy, dynamical and static light scattering, small-angle neutron and X-ray scattering, magnetometry, magneto-rheometry) of MCFs and their use in engineering devices will be summarized.

Plenary Pl-17

Nanostructured black silicon fabrication for energy conversion

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Abstract. Silicon as an earth-abundant element has been widely used in microelectronics and microsystems. Nanostructured silicon machined by dry or wet chemical etching are normally shows high absorption for visible light and exhibits “black” colour (so-called black silicon). Such behaviour is originated from suppressed reflection and scattering of micro/nanostructured surface morphology. The micro/nanostructure surface traps visible light energy through internal multi-reflection, scattering and light-matter coupling. Only a few photons of incident light can escape from the surface. In this presentation, with the help of metallic nanoparticles-induced plasmon effect and geometric configuration, we demonstrate that infrared light wavelength photons end up being captured as well. Theses micro/nanostructures can efficiently facilitate dissipation of light energy into electricity and heat. The nanostructured black silicon is becoming a new favourite in the fields of solar cell, photodetection, bio-imaging and security warning applications.

Section T1:

Stable Isotopes, Labeled Compounds and Analytical Techniques

Oral T1-1

Method for determination of sulfur content: Analytical characterization and application to acid mine drainage water samples

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Abstract. Presence of sulphide minerals in mining wastes represents an important environmental concern due to its crucial role in the acid mine drainage formation. The aim of the study is to evaluate the analytical characteristics of an optical emission capacitively coupled plasma microtorch spectrometer coupled with a small size electrothermal vaporization device (SSETV-μCCP-OES) for determination of sulfur content in acid mine drainage. The advantages of the method compared to classical laboratory instrumentation such as inductively coupled plasma optical emission spectrometry or mass spectrometry (ICP-OES, ICP-MS) are cost effectiveness, low power and Ar consumption, simplicity and, for water sample analysis, there is no need of sample preparation, as the electrothermal set up is not affected by small particle presence that could clog the nebulizer used in ICP-OES/MS. These characteristics make the proposed method suitable for the determination of total sulfur content in acid mine drainage water samples.

Oral T1-2

New approach in food analysis

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Abstract. These days, the open circulation of food products and the large interest of customers for good-quality and authentic products made the development of reliable, rapid and cost-effective methodologies, able to discriminate between various categories, to become a priority, both for the research community and control entities. Among these methodologies, the combination between Raman spectroscopy and Machine Learning algorithms allowed an efficient identification and classification of several food and beverages. This work discusses the necessities and the efficiency of this methodology in analysing several food and beverages as edible oils, honey and fruit spirits with respect to trademark or their geographical and botanical origin. Thus, the results and the potential of these achievements for food authentication and control are explained considering each matrix particularity and complexity. **Acknowledgment**: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number 260PED/2020, within PNCDI III*

Oral T1-3

Evaluation of heavy metal contamination in *Mytilus* sp. using fast detection physico-chemical methods

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Abstract. Shellfish has become more popular in our diets, own to the many benefits provided to human health. However, especially in the case of molluscs, there is a strong possibility of heavy metal contamination, especially since costal waters might be highly polluted. The existing detection methods involve sophisticated chemical protocols. To address this issue, we proposed the use of fast detection of contaminants based on energy dispersive X-ray spectroscopy. The results obtained with this method were well corelated with the more sensitive X-ray fluorescence spectroscopy. In the same time, the structure of the shells was analysed and results were correlated. Overall, the method proposed shows very good premises for the fast and reliable detection of heavy metal contamination in shells.

Oral T1-4

The opportunities of in situ XAS and XRD for monitoring the dynamics of complex systems

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Abstract. Within the framework of energy and environmental applications, understanding the structure origin of novel material properties, the reaction mechanisms in the photoelectrochemical process, the nucleation and growth kinetics of novel materials, etc. are of great interests for fundamental and technological researches. However, the characterization of these complex systems is still great challenge. Here, in situ X-ray absorption spectroscopy and X-ray diffraction, are used in the investigating complex systems. Using several representative examples, we illustrate the role of in situ techniques in the characterization of new details about the growth process of organic-inorganic hybrid perovskite, the catalytic reaction mechanisms of nanoceria, also the relationship between the structure and properties of electrocatalytic materials. Following this approach it is possible to design and prepare novel materials.

Poster T1-1

Determination of capsaicin and dihydrocapsaicin in topical creams using HPLC and extended standard addition calibration

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Abstract: Capsaicin and dihydrocapsaicin, the pungent principles that account for 90% of total capsaicinoid content in chilli peppers, are lipophilic alkaloids formed through the condensation of vanillylamine with fatty acid derivatives, that only differ in the saturation of the fatty acid moiety. Capsaicin has been explored therapeutically, in the field of pain management, due to its ability to bind the TRPV1 receptor. Applied topically, capsaicin may desensitize the skin, by inducing a loss of nociceptor fiber function. In this study, a method for the non-destructive determination of capsaicin and dihydrocapsaicin from topical creams is developed. The method involves subsequent solvent extractions of capsaicinoids from topical creams, and HPLC analysis of the further processed pooled organic fractions. The relative peak area for each analyte serves as the dependent variable in the calibration study. Extended standard addition was chosen as calibration methodology, since this approach also takes into account the linearity of the calibration function below spiking level zero. The method was evaluated in terms of dynamic range, limit of detection, precision and accuracy, and then used to calculate the confidence intervals for the mean capsaicin and dihydrocapsaicin content of real samples (3 types of commercially available topical creams containing *Capsicum* extracts). **Acknowledgements**: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number TE-2019-1396, within PNCDI III.

Poster T1-2

Reactors for sulfuric acid decomposition in the thermochemical production of hydrogen

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Abstract. In the thermochemical cycles: S – I, S – Br hybrid and S – hybrid, for hydrogen production, the decomposition of sulfuric acid represents the step with biggest energy consumption, according that the process takes place only at high temperature in the presence of a catalyst. The sulfuric acid conversion has two steps: - Thermal decomposition: $H2SO4(l) \rightarrow SO3(g) + H2O(g)$; $\Delta H = 97.54$ kJ/mole; (~ 400oC) and Thermo-catalytic conversion: $SO3(g) \rightarrow SO2(g) + 1/2O2(g)$; $\Delta H = 98.92$ kJ/mole; (850 – 900oC, catalyst). Besides the fact that the temperature required for those two reactions must be ensured, due to the extremely corrosive reaction medium (SO2, SO3, H2O vapors, O2, H2SO4 unconverted) special materials must be used to make the reactors. A silicon carbide reactor, having a honeycomb structure, on which an iron trioxide layer was deposited as a catalyst, heated by means of solar radiation, is presented. The conversion of sulfuric acid at pressure was also studied using an installation composed of: evaporator, conversion reactor, condenser and a condensate collection vessel; the first two were made from Hastelloy C-276. It is also presented a conversion reactor in the form of a bayonet type heat exchanger, made of silicon carbide.

Poster T1-3

Compensation effect in catalytic oxidation of carbon monoxide

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Abstract. The compensation effect in heterogeneous catalytic reactions is linked with appropriate change in the activation energy. If a linear relationship between activation energy and pre-exponential factor or activation enthalpy and entropy take place for a reaction in present of different catalysts, a compensation effect is expected. Compensation effect has been incompletely investigated as a method for quantitative comparisons of catalytic activity in different systems. This study aims to identify the occurrence of the compensation effect in CO oxidation reaction to CO_2 catalyzed by Pd/Al_2O_3, Ni/Al_2O_3, CuO/Al_2O_3 and Ni/TiO_2

Poster T1-4

Dual-mode determination of selenium in biofortified *Allium* microsamples following piazselenol formation and solid phase microextraction

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Abstract. Selenium is an essential trace element naturally distributed in all compartments of the environment. Compared to other micronutrients, there is a much thinner line between the normal concentration and the toxic amount of selenium in living organisms. The inorganic forms of selenium (selenate, selenite) present up to 40 times higher toxicity than its organic combinations (e.g. selenocysteine, selenomethionine). This is why a sensitive method is required for detection of selenium species in biological samples. A distinct method is represented by the formation of piazselenol. This kind of complexes represent the product of reaction between an aromatic o-diamine and Se(IV) species, in acidic conditions. This study describes an HPLC-based optimized, sensitive and selective method for determination of selenium in biological microsamples. Molecular absorption UV-Vis analysis of piazselenol formation has also been carried out, using a nanophotometer device, as a faster but still efficient assay for selenium determination in microsamples. Before the analysis procedures, the biofortified Allium microsamples have been mineralized and pre-concentrated using solid-phase microextraction technique which affords an excellent precision and accuracy as it removes the interferences form a typical biological sample, allowing thus limit of detection as low as 0.5 ng/mL Se. **Acknowledgement**. This work has been financially supported by PN-III-P1-1.1-TE-2019-1396.

Poster T1-5

Analysis of the painting materials from the Dângău Mic wooden church, Cluj County

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Abstract. The wooden church from Dangaul Mic village was built in 1764 and still preserves the original painting from 1802. The architecture and beautiful interior frescoes make this Transylvanian church a part of the national heritage of Romania, being a historical monument. Such churches are in danger of degradation due to their age and lack of interest of the local authorities for their conservation and restoration. In order to preserve the information regarding the current state of the church, which will facilitate future restoration efforts, a detailed investigation of the painting materials was carried out as well as imagistic documenting. Analyses were performed by X-ray (XRF) spectroscopy and destructive and non-destructive Fourier transform infrared (FTIR) spectroscopy.

Poster T1-6

Investigations regarding helium isotopes separation by gas chromatography

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Abstract. Helium-3 is a gas with properties that currently make it in high demand. There are several applications that require the use of helium-3 use, ranging from neutron detection till medicine, industry and science. The helium-3 isotope is produced by beta disintegration of tritium. An important source of helium-3 is the cover gas used in the moderator circuit at Cernavoda NPP. The objective of this paper is to propose a method for the investigation and evaluation of the separation and recovery of helium isotopes by gas chromatographic method. The chromatographic column used for this study is a packed, 5 meters long column filled with 5A molecular sieve, using hydrogen as carrier gas. The column is operated at 77K and different carrier gas flow rates in the range of 20 – 90sccm.

Poster T1-7

Assessment of *trans* fatty acids content in food from Romanian market

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Abstract. *Trans* fatty acids are chemically "monounsaturated" or "polyunsaturated". They are considered so different from the *cis* monounsaturated or polyunsaturated fatty acids that they can't be legally designated as unsaturated for purposes of labelling. Gas chromatography (GC) and infrared spectroscopy (IR) represent two complementary methods most commonly used to identify and quantify *trans* fatty acids. The law in Romania (No. 182/2020) requires that *trans* fats content is included in labelling of food and not exceed 2g/100g of fat. The quantitation and identification of *trans* fatty acid isomers by GC is difficult because of the wide range of fatty acid isomers present in complex food samples. Accurate information on the content of *trans* fat in foods can come from proper techniques for extracting lipids, saponification, and methylation of fatty acids. The GC-FID technique was used for detection, separation, identification and quantification of *trans* fatty acid in food. Lipids were extracted from the food and fatty acids converted into methyl esters and analysed by GC. In addition, the FT-IR method for rapid screening of *trans* fats was proposed. **Acknowledgments:** The financial support for this work was provided by the PN-III-P2-2.1-PED-2019-3502 Program, Project number 354PED/2020 ("Assessment of content and distribution of *trans* fatty acids in food products from Romanian market"). The project was supported by the UEFISCDI.

Poster T1-8

Assessing the isotopic fingerprint of ethanol from Transylvanian distillates

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Abstract. Romania has an old tradition in production of fruit spirits. The authentication of distillates is an important research field because their composition has a considerably higher variation than the one of beer or wine, whereas numerous raw materials are permitted in production process. Isotopic fingerprints of ^{2}H and ^{18}O were determined by high temperature pyrolysis system coupled to an isotope ratio mass spectrometer (IRMS). All isotopic measurements were made on the ethanol recovered after fruit spirits distillation. Extraction of ethanol was obtained using a Cadiot spinning band column. The remaining water was trapped by preserving the distillate for 48 h on a molecular sieve. The data set consisted in 50 fruit distillates, coming from Transylvania, Romania, produced from plums, apples, pears, apricots and quinces. The variation range was between 7.9 ‰ and 21.7 ‰ for $\delta^{18}O$, and between -228.0 ‰ and -160.2 ‰ for $\delta^{2}H$, respectively. **Acknowledgment**: T*his work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number 260PED/2020, within PNCDI III.*

Poster T1-9

Multielement analysis of fruit distillates from Transylvania area

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Abstract. Distilled beverages are important for both consumers, as well as for producers. Traditional methods and innovative technologies in fruit distillates production are focusing on their quality improvement. In recent years, the application of analytical methods for the quality assessment, classifying beverages according to origin or for the trademark specific fingerprinting has attracted increasing attention of researchers. Fifty fruit distillates ranging in alcoholic degree 40 and 80 from different regions of Transylvania were investigated from the elemental profile point of view using Inductively Coupled Plasma Mass Spectrometry (ICP-MS). The statistical analysis, based on the multielement content was applied in order to find which of the metals represents the best markers for: i) the geographical origin of samples; ii) the trademark specific fingerprinting; iii) the fruit varieties differentiation which were used for fruit distillates. **Acknowledgements:** This work was supported by Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI), through the project 260 PED/2020, within PNCDI III.

Poster T1-10

Mushroom's evaluation based on FT-IR fingerprint and chemometrics

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Abstract. Mushrooms are macrofungi that represent an important source of vegetarian proteins, along with other bio-active molecules. Infrared spectroscopy provides a non-destructive measurement, user-friendly, which is able to assess the presence of bio-active compounds within minutes, thus becoming suitable for classification purposes, where a large data set is needed. For this study three mushroom species grown in Romania, were selected namely, *Armillaria mellea* (12 samples), *Boletus edulis* (31 samples) and *Cantharellus cibarius* (34 samples). For highlighting the subtle differentiations that occurred in the obtained IR spectra, some chemometric methods were applied: principal component analysis (PCA), linear discriminant analysis (LDA) and k nearest neighbour (kNN). This approach (IR spectra combined with chemometric interpretation), provided good classification models. The most representative IR region was assigned to α-glucans and β-glucans, whose beneficial effect upon human health is well known: immunomodulatory, antitumoral, hipolipidemic and antimicrobial. **Acknowledgments**. The financial support for this work was provided by Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI), through the project PD 90/2020.

Poster T1-11

Spectrophotometric methods used for investigation of total phenolic compounds and antioxidant activity of commercial edible oils

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Abstract. Edible oils are widely used by food industry due to their nutritional properties and their influence on the smell and taste of food products. Olive oil, especially extra virgin olive oil has nutritional and sensory characteristics that make it unique and a basic component of the Mediterranean diet. Its importance is mainly attributed to its richness in polyphenols, which act as natural antioxidants and may contribute to the prevention of several human diseases. In this work 55 commercial edible oils (41 samples of olive oil and 14 of sunflower oils) were investigated from total phenolic compounds (TPC) and antioxidant activity (AA) point of view. The Folin-Ciocalteu colorimetric method was used for TPC determination in oil samples and spectrophotometric DPPH (2,2-diphenyl-1-picrylhydrazyl) method for AA, respectively. The obtained DPPH values for methanolic extract of olive oils ranged between 4.72-31.40 mg Trolox/100g and 2.06-3.96 mg Trolox/100g for sunflower oils, respectively, while for the TPC were between 4.65-26.39 mg gallic acid/100g for olive oils and 0.28-0.91 mg gallic acid/100g for sunflower oils. **Acknowledgment**. The financial support for this work was provided by Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI), through the project 354 PED/2020.

Poster T1-12

Synthetic Strategies for Labeled Catecholamine-Based Compounds

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Abstract. In this paper we present the recent results in synthesis and structural analysis of some isotopically labeled catecholamine derivatives, in order to elucidate aspects of their polimerization process. The selective labeled intermediates with ^{15}N and ^{13}C are required in order to reduce the obstacles encountered in deciphering the mechanism of polydopamine and its analogues formation. Consequently, it was proposed the selective synthesis of ^{15}N and ^{13}C labeled key-compound 3-amino-2-(3,4-dihydroxibenzyl)-propionamide using a multi-step strategy that follows both known literature data and also modified procedures.

Poster T1-13

Applications of ANNs in honey recognition based on isotopic and elemental content

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Abstract. Nowadays, an important help for control laboratories is given by the development of reliable tools for experimental data processing in order to build advanced recognition models for distinct food commodities. This work discussed in detail the opportunities and limitations of Artificial Neural Networks (ANNs) for honey recognition. Therefore, the isotope and elemental content determined through IRMS - Isotope Ratio Mass Spectrometry and ICP-MS - Inductively Coupled Plasma Mass Spectrometry, respectively were used as markers for the model development. This approach conducted to the development of a prediction model for geographical recognition having an accuracy of 96.27% while for the floral differentiation a lower percentage was recorded because the used markers are acknowledged predictors for geographical recognition rather than for botanical identification. **Acknowledgment**: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number 7PCE/2021, within PNCDI III*

Poster T1-14

Kinetics and thermodynamics for U(VI), Fe(III) and Cr(VI) adsorption using an anion exchange resin

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Abstract. In the present study, a comparison was made between uranium (VI), iron (III) and chromium (VI) adsorption from different solutions, onto Dowex-Marathon resin. In order to investigate the kinetic mechanism which controls the adsorption, four kinetic models were used: pseudo-first order, pseudo-second order, Elovich equation and intraparticle diffusion model. The thermodynamic parameters such as the Gibb's free energy ($\Delta G°$), the standard enthalpy ($\Delta H°$) and the standard entropy ($\Delta S°$) were determined indicating that all the mentioned ions adsorption process was spontaneous and endothermic. Our target is to found materials to be in agreement with the world's growing interest in wastewaters treatment.

Poster T1-15

Trans fat content in edible oils commercially available in Romania

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Abstract. *Trans* fatty acids are formed industrially through partial hydrogenation of unsaturated fatty acids in vegetable and marine oils. The purpose of this hydrogenation is to produce fats with improved oxidative and thermal stability as well as modified physical properties. During industrial hydrogenation of the vegetable oils, apart from getting converted into saturated derivatives, some of the unsaturated fatty acids are also converted into *trans* isomeric forms. The profiles of *trans* fat from commercially available oils and natural resources are not the same. This study describes an analytical method developed for the separation, identification and quantitation of *trans* isomers of unsaturated fatty acids. The fatty acid composition is determined as the methyl esters of fatty acids by GC–FID. This method is applicable to a wide variety of food matrices, with particularly emphasised analysis of *trans* unsaturated fatty acids in oils. **Acknowledgments:** The financial support for this work was provided by the PN-III-P2-2.1-PED-2019-3502 Program, Project number 354PED/2020 ("Assessment of content and distribution of *trans* fatty acids in food products from Romanian market"). The project was supported by the UEFISCDI.

Poster T1-16

Determination of the Fatty Acids profile in edible oils using GC-MS system

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Abstract. Fatty acids are an important structural and functional component of edible oils and their individual composition is the main determinant of oil quality. The profile of the fatty acids (FAs) classes as saturated (SAFA), monounsaturated (MUFA) and polyunsaturated (PUFA) is relevant from the nutritional point of view. The presence of saturated fatty acids in meat products is associated to an increased incidence of cardiovascular diseases and the polyunsaturated with risk for cancer dieses. Therefore the determination of FAs structures in foods is relevant in the development of strategies for a healthy diet. In this work, a simple and sensitive method based on coupled system Gas Chromatograph-Mass Spectrometer (GC-MS) for the simultaneous determination of saturated and unsaturated FAs in edible oils is described. **Acknowledgments:** *The financial support for this work was provided by the PN-III-P2-2.1-PED-2019-3502 Program, Project number 354PED/2020. The project was supported by the Executive Unit for Financing Education Higher R&D and Innovation, UEFISCDI.*

Poster T1-17

Fatty acid and multielement profile of breast milk over different lactation stages

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Abstract. Breast milk represents the best food available for infants. Exclusive breast feeding is recommended for the first 6 month of life. Breast milk consists mainly of water, carbohydrates, lipids, proteins, vitamins and minerals. Lipids can account for only about 4% of breast milk, but the composition of *cis* fatty acids is one of their major components. The profile of fatty acids is influenced by various factors, such as: maternal age, stage of lactation, composition of maternal diet, etc. growth and development. In particular, *trans* fatty acids (TFAs) in human breast milk have raised concerns because of the possible adverse effects on infant's growth and development. The aim of our study was to evaluate the changes in fatty acid composition and multielement profile of breast milk over lactation stages. Fatty acid methyl esters were separated and quantified by GC-FID. Concentrations of macro, micro minerals and potentially toxic metals were analysed by ICP-MS. **Acknowledgments:** The financial support for this work was provided by the PN-III-P2-2.1-PED-2019-3502 Program, Project number 354PED/2020 ("Assessment of content and distribution of *trans* fatty acids in food products from Romanian market"). The project was supported by the UEFISCDI.

Poster T1-18

Fractional distillation column design for hydrogen isotope separation

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Abstract. Fractional distillation of hydrogen isotopes through cryogenic distillation is the most productive process to enrich and recover tritium. In combination with Combined Electrolysis Catalytic Exchange process, form the full technology to detritiate low level tritiated water and tritium recovery within any application. The aim of this work is to present the design of a fractional distillation column for hydrogen isotope separation through cryogenic distillation to be connected to the CECE process developed at ICSI Pilot Plant. This is done by using a software developed "in house", based on heat and mass transfer model. Based on the input data like, flow rates, composition of the feeding gas, pressure drop, the simulation provides the distribution of all the molecular species involved, temperature profile and also the liquid and vapor enthalpies along the column.

Poster T1-19

Fuzzy algorithms applied in fruit spirits authentication

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Abstract. The development of analytical approaches based on distinct types of spectroscopies in corroboration with either advanced chemometric models or artificial intelligence represents nowadays a priority for research and control laboratories, in the attempt to develop efficient tools for adulteration detection of food and beverages. The choose of the optimum data processing method, is important issue in the development of reliable models for alcoholic beverages differentiation. In order to prospect the efficiency of the application of ^{1}H-NMR spectroscopy in conjunction with Fuzzy algorithms, in this study a fruit spirits sample set were employed, for different classifications. The ^{1}H-NMR measurements were recorded in buffered D_2O solution and all chemical shifts were measured relative to TSP (3-(trimethyl-silyl)-propionic acid sodium salt), added as internal standard referencing the chemical shift to 0 ppm, applying water suppression pulse program for irradiation of the water signal. **Acknowledgement.**. This work was supported by Romanian National Authority for Scientific Research and Innovation (UEFISCDI), through the project 260 PED-2020, within PNCDI III.

Poster T1-20

Applications of stable isotopes for geographical and varietal recognition of Romanian and French honeys

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Abstract. Honey is one of the most falsified food commodities in the world and for this reason, the development of new and reliable analytical approaches, able to differentiate among distinct honey origins and varieties, represents a continuous preoccupation among researchers and control laboratories. The research towards the identification of new authenticity markers is crucial to fight against fraudulent activities on honey, one of the top ten most falsified food commodities. This work proposes an association of stable isotopes and elemental content as markers for honey authentication, with respect to its floral and geographical origin. Emerging markers like isotopic signature of honey water were used to develop new recognition models. Thus, the efficiency of the discrimination potential of these emerging markers was discussed individually. *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PCE 7/2021, within PNCDI III.*

Poster T1-21

Synthesis and Structural Analysis of Some Isotopically Labeled Amadori Products

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Abstract. Amadori rearrangements are milestone reactions of carbohydrate chemistry, mainly because these products combine the structural characteristics that derived from both core units, an aminoacid unit and a carbohydrate unit. The aim of this work was the synthesis of some Amadori products following a multi-step strategy and using some isotopically labeled aminoacids, which further, could act as building-blocks in synthesis of some biomolecules (e.g. glycopeptides).

Poster T1-22

Optimization of nitrogen-15 production by isotopic exchange in nitrox system

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Abstract. The main aim of this study was to optimize the operating parameters for ^{15}N producing plant, used at the National Institute for Research and Development of Isotopic and Molecular Technologies from Cluj-Napoca, for high-level enrichment of nitrogen -15 by isotopic exchange reactions between nitrogen oxides (NO, NO_2) and aqueous solution of nitric acid (HNO_3). The optimization was based on the theory of ideal cascades applied for square cascades. The theoretical results were compared with experimental data obtained in total reflux conditions, using the final column of the ^{15}N producing plant. Good agreement was obtained between the predicted optimized operating conditions and the experimental data results.

Poster T1-23

Finding best weighted linear regression model for heteroscedastic data by maximizing likelihood function

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Abstract. Ordinary least squares regression (OLS) is the most frequently used method applied in analytical chemistry for estimation of the parameters of a calibration curve. Most important assumptions in OLS regression presume a linear data set, little or no error for independent variable, independence and normal distribution of the residuals, no outliers and last but not least constant variance or a homoscedasticity. A dataset whose variance of the residuals depends upon the independent variable is called heteroscedastic as to oppose to homoscedastic ones. Residuals plots or statistical tests such as Breusch-Pagan or White test are commonly used for diagnosing a heteroscedastic behavior. However, these tests are not efficient if the dataset is low in size. If the dataset is proven to be heteroscedastic, weighted linear regression, log transformation or nonparametric median regression could be applied instead. In the context of a weighted linear regression, it is necessary to choose a suitable weight that leads to the best predictive model and most frequently is used a weight like 1/x, 1/x2, 1/x1/2 or generally 1/xγ. In this presentation, a novel way to estimate the best weight for weighted linear regression will be presented using the profile of the log-likelihood regression function. Moreover, this method appears to be a goldfish since not only indicates the most appropriate weight but also diagnose the heteroscedastic profile and variance non-homogeneity along the x axis. **Acknowledgements**: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number TE-2019-1396, within PNCDI III

Poster T1-24

Investigation of the painting of the royal icon of Jesus Christ

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Abstract. The royal icon of Jesus Christ belongs to the Saint Archangels Michael and Gabriel church from the village of Gheorgheni, the municipality of Feleacu, county of Cluj; it dates from the 18th century and was painted in 1702 by Vasile Zugrav – an icon artist from Saliste, the county of Sibiu. Considering the importance, the age and the process of restoration of this icon, researches have been done to establish the composition of the painting materials. These have been made using non-invasive FTIR and XRF investigations for each color in different points.

Poster T1-25

The spectroscopic analysis of constituent materials of the Romanian icon, "The Entry of Lord into Jerusalem", by Grigore Ranite

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Abstract. Grigore Ranite is an important painter in the orthodox religious art of the eighteenth-century. The purpose of this in-depth analytical investigation was to study the materials and the techniques used by the artist to "write" the icon, "The Entry of the Lord into Jerusalem", which is in the Ethnographic Museum of Transylvania. Particular attention was dedicated to obtaining information about the degradation of the ancient materials used in the icon. To achieve this aim a multianalytical approach was used, including Fourier Transform Infrared (FTIR) and X-ray fluorescence (XRF). The traditional technique of "writing" icons led to a distribution into more layers of inorganic and organic materials and these generated very complex spectroscopic spectrums. The second derivate IR spectrum has allowed a better resolution of the bands specific to functional groups, corresponding to the components of the materials.The results of the investigation will help to enrich the knowledge of Romanian art and also help in any future restoration and conservation work.

Poster T1-26

Concentrations and exposure risks of toxic elements in facial cosmetics

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Abstract. The analysis of cosmetics constitutes a challenge mainly due to the large variety of ingredients and formulations, leading to vast matrix complexity and variability. The concentrations of heavy and toxic metals were determined in facial cosmetics from the Romanian market. The study was aimed to provide information on the risk associated with human exposure to metals in these facial cosmetic products. The concentrations of metals in the samples were measured by ICP-MS spectrometry according to the two steps temperature-controlled digestion program Microwave Digestion. The risk characterization was performed by calculating the systemic exposure dosage (SED). The results showed that the heavy metals exposure through the usage of these facial cosmetic products is below their respective provisional tolerable daily intake (PTDI) or recommended daily intake (RDI) values. The heavy metals levels in the investigated facial cosmetics present no potential risk to the users' health.

Section T2:

Molecules, Biomolecules and Green Technologies

Oral T2-1

Low-lying electronic excited states of dopamine

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Abstract. The low-lying electronic transitions induced in dopamine molecule have been investigated considering UV-VIS and time resolved spectroscopy techniques as well as advanced quantum mechanics methods. The experimental absorption and fluorescence spectra are compared with the theoretically computed excited state electronic energies obtained using time dependent density functional theory (TDDFT) and equation-of-motion-like coupled-cluster (STEOM-DLPNO-CCSD) method and considering the def2-TZVP triple-ξ quality basis set. The nature of different electronic transitions in terms of the orbitals configurations is also discussed.

Oral T2-2

The perspectives of NMR and artificial neural networks analysis used for an advanced medical diagnosis

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Abstract. An artificial neural network (ANN) is defined as a numeric machine able to learn by examples and eventually to perform complex tasks. The trained ANN becomes capable to process rapidly large amounts of data in order to solve problems for which it is difficult to provide a simple-model solution, and eventually can give an educated prediction in real time. While ANNs are commonly implemented for image recognition, speech recognition or posture recognition, we will discuss the use of an ANN to analyse NMR data in order to obtain an educated medical diagnosis. The general architecture of an ANN and the simplest implementation into a program written in JavaScript using the machine learning library **ml5** version 0.4.3 are presented. Finally the application of ANN to cancer classification is largely discussed. For that, a preliminary principal component analysis (PCA) of a data set of three groups of *in vivo* ^{1}H NMR spectra recorded for 52 uterus specimens (healthy, with endometrial cancer and with uterine cervical cancer) was performed. The PC1 versus PC2 was used for medical diagnosis.

Oral T2-3

Spectroscopic evaluation of vitamins effect on the BSA - LT4 complex

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Abstract. The bioavailability of administered drugs that reach the systemic circulation depends on the pathology and diet of the patient. Bovine serum albumin (BSA) acts as a carrier for many endogenous and exogenous compounds, such as levothyroxine (LT4) or other drugs. LT4 is essential to treat hypothyroidism and dietary supplements such as vitamins can influence the BSA-LT4 interaction. In this study, the interaction between LT4 and BSA, as well as the effect of vitamin C, vitamin B12, and folic acid (FA) on the BSA-LT4 complex were investigated using fluorescence, Surface Plasmon Resonance and UV-Vis spectroscopy. Experiments showed that LT4 interacts with BSA mainly by a static mechanism. The binding is a spontaneous process, induced by van der Waals forces and formation of hydrogen bonds. The thermal stability of the BSA-LT4 complex is more pronounced in the presence of FA and vitamin B12, while vitamin C does not influence the stability of BSA-LT4 complex. Of the three vitamins, vitamin B12 binds with high affinity to the site of the protein already bound with LT4. In this way, vitamin B12 stabilizes the BSA-LT4 complex, and the immediate effect will be to decrease the concentration of free LT4.

Oral T2-4

Novel Antimicrobial Peptides: *In silico* Design and Experimental Validation

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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 small host defensive peptides with high selectivity of interaction with bacterial cells over mammalian cells. Here we propose a 3-stage *in silico* AMP design approach using molecular docking, molecular dynamics and potential of mean force calculations. The aforementioned approach suggested new antimicrobial peptide candidates, whose activity against bacterial cells / toxicity against mammalian cells were further tested by means of three complementary experimental approaches (microbiology, surface-enhanced Raman spectroscopy, atomic force microscopy). In the end, at least one novel antimicrobial peptide was identified. Moreover, this novel AMP has presented no inhibitory effects on tested human cells, a crucial aspect in developing novel AMPs.

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Oral T2-5

The evidence of microplastics in karstic spring waters and their characterization using Raman Spectroscopy

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Abstract. The growing use of plastics has been accompanied by an increase of plastic waste in the environment and grown into a global problem. Macro-plastics aging generates a multitude of secondary microplastic fragments. The pollution with microplastics of large waters bodies such as rivers, seas and oceans was already proven, but the presence of microplastics in karstic springs was poorly studied. Karstic spring water is frequently used for its purity against pollutants but this work will point out that this is no longer the case. In this study, Raman Spectroscopy was used to confirm the presence of microplastics in the spring waters collected from rural areas (Josani and Albioara) in the Apuseni Mountains, Western Romania. A volume of 1000 l of water were filtered through six sieves with the mesh dimensions of 20, 45, 63, 100, 250 and 500 μm. The particles retained on the sieves were transferred to Millipore filters , microplastics sorted and examined under light microscopy and Raman micro-spectroscopy, respectively. An interesting accumulation of blue microplastics was noted on all filters, among other transparent, white and red microfragments. The results unambiguously confirm the presence of common microplastics in karstic spring waters and provides information about the type of microplastic and their pigment.

Oral T2-6

The strength of enzymes in polymerization reactions of α-hydroxy acids

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Abstract. Polymers are used ubiquitously in a wide range of industrial applications ranging from structural materials to electronics and in our daily life from chopsticks to trash bins due to their diverse functionality, lightweight, low cost, and excellent chemical stability. Polymerization of α-hydroxy acids can be achieved by polycondensation and self-polycondensation, by ring-opening polymerization or enzymatic process. This work focuses on the behaviour of three α-hydroxy acids: tartronic, tartaric, and 4-hydroxymandelic acids in the enzymatic conditions. An enzymatic polymer synthesis has the following outcomes: perfect control of polymer structures, creation of polymers with a new structure, a clean, selective process without by-product formation, a low loading process with energy saving. Their structure and particularities will be compared with the previously reported thermal-polycondensation method for which analytical techniques such ss-NMR, mass spectrometry or FTIR spectroscopy are the keys to underline their polymeric matrix.

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Oral T2-7

Mechanochemical Synthesis of Corannulene Derivatives

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Abstract. Corannulene ($C_{20}H_{10}$) is a polycyclic aromatic hydrocarbon that exhibits molecular curvature due to the arrangement of five six-membered rings around a central five-membered ring (Figure 1). It can, therefore, be considered as the cap region of fullerene C_{60}. This is the reason corannulene is sometime referred to as a 'buckybowl'. The nonplanarity of the structure endows corannulene (and C_{60}) with unique electronic properties that are not found in planar aromatic hydrocarbons such as anthracene and pyrene. In contrast to C_{60}, however, corannulene offers high solubility in common organic solvents and an avenue for multiple and well-defined substitutions on the aromatic nucleus. These two attributes are of high relevance to the synthetic and materials chemists as they allow for synthesis and unambiguous structural characterization of the synthesized materials. In this presentation, we will discuss our synthetic work relating to mechanochemical synthesis of corannulene and its derivatives.

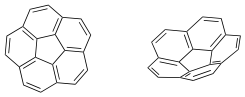

Figure 1. Chemical structure of corannulene.

Oral T2-8

Ligand-induced conformational signals in kinase networks

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Abstract. Rho-associated protein kinase 2 (ROCK2) is a membrane-anchored, long, flexible, multidomain, multifunctional protein. Its functions can be placed into two categories: membrane-proximal and membrane-distal ones. A recent study concluded that membrane–distal functions, e.g. regulatory myosin light chain (RMLC) phosphorylation requires a fully extended conformation, and this conclusion was supported by electron microscopy. The present solution small angle X-ray scattering (SAXS) study revealed that ROCK2 population is a dynamic mixture of folded and partially extended conformers. We have shown that the predicted, auto-inhibited, folded conformation of ROCK2 exists in solution, and is stabilized by weak non-covalent interactions between the N- and C-termini. Binding of RhoA to the coiled-coil domain shifts the equilibrium towards the partially extended state. The binding of natural protein substrates (e.g. LIMK1) to the kinase domain breaks up the interaction between the N-terminal kinase and C-terminal regulatory domains, but smaller substrate analogues do not. The present studies reflect the dynamic behaviour of this long, dimeric molecule in solution, and our structural model provides a mechanistic explanation for a set of membrane-proximal functions, while allowing for the existence of an extended conformation in the case of membrane-distal functions.

Poster T2-1

Identification and quantification of valuable bioactive compounds from three commercial species of Stachys

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Abstract. The aim of this research is to investigate three species of Stachys (S. lavandulifolia, S. officinalis and S. germanica) in terms of polyphenol concentration, volatile compound content and their antibacterial activity. The antibacterial activity focused on investigations on the bacterial strains present in human pathology, namely: Enterobacter faecalis, Escherichia coli, Clostridium perfringens, the method used being the Kirby-Bauer diffusimetric method. In conclusion, it can be stated that the studied plants (S. lavandulifolia, S. officinalis and S. germanica) can be recommended in alternative medicine by having a series of bioactive and antimicrobial qualities.
Acknowledgments: Project PN 19110302 "Research on the variation trends specific to stable isotopes in different tree species: deepening the fractionation mechanisms and the chemical processes interconnected on the soil–water–plant chain".

Poster T2-2

Spectral analysis of Laurdan fluorescence reveals changes induced by AMPs in lipid membranes

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Abstract. Antimicrobial peptides (AMPs) are a class of molecules synthetized by various organisms with the aim of protecting themselves against pathogens. In order for the peptides to enter the cells they have to pass or interact with the plasma membrane. The effects of various peptides at the lipid membrane level were investigated using Laurdan fluorescence. Laurdan, a lipid membrane probe, is sensitive to polarity changes in the environment. The fluorescence spectra were interpreted using the classic generalized polarization (GP) parameter, as well as using the previously described log-normal deconvolution. The later method allowed us to infer other parameters: the difference between the relative areas of elementary peak (ΔSr), and the ratio of elementary peaks areas (Rs). The parameters analysed allowed us to highlight different changes induced by the peptides investigated.
Acknowledgements: This work was supported by the Romanian Ministry of Research, Innovation and Digitization, through the National Core Program No. PN 19 06 02 03/2019;

Poster T2-3

Effect of gamma radiation on some dosimetric interest compounds: an EPR study

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Abstract. The present research was undertaken in order to investigate if some compounds used as natural sweeteners (steviol and sucrose) can be used as EPR dosimeters. The samples were exposed to low doses of gamma ionizing radiation used in the practices of radiodiagnostic medicine and interventional radiology. The EPR spectra of the γ-irradiated compounds reveal large signals, with multiple lines, which are characteristic for the free radicals in the solid state. From the analysis of the dependence of EPR signal of the absorbed dose, it was observed that by γ - irradiation the amount of generated radicals shows a linear dependence, which mean that there exist a possibility to use these two compounds as EPR dosimeters.

Poster T2-4

Investigation of Citronella Oil as Green Corrosion Inhibitor for Carbon Steel in Acidic Media

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Abstract. Corrosion inhibition of carbon steel (C-steel) in acidic media was investigated in the absence and presence of different concentrations of plant oils. The aim of the present work is to prevent corrosion of carbon steel and the goal was achieved and confirmed by using the naturally occurring, low-cost and environment-friendly inhibitor Citronella Oil. A set of techniques was used for samples preparation (Drop-Casting) and investigation (Open Circuit Potential (OCP), Linear Polarization (LP), Tafel plots and Electrochemical Impedance Spectroscopy (EIS)). The metal surface morphology before and after corrosion tests were also investigated by: Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS) and Atomic Force Microscopy (AFM). **Acknowledgements**: The present work has received financial support through the project: Entrepreneurship for innovation through doctoral and postdoctoral research, POCU/360/6/13/123886 co-financed by the European Social Fund, through the Operational Program for Human Capital 2014-2020.

Poster T2-5

PAMAM dendrimers conjugated with antimicrobial peptides

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Abstract. Antimicrobial peptides (AMPs) are potential next-generation antibacterial agents, less prone to bacterial resistance. Dendrimer-based delivery systems such as polyamidoamine (PAMAM), offer new routes to improve and control the drug delivery. In order to address the particularities of antimicrobial therapies, we have produced stable, non-covalent PAMAM-AMP conjugates. The binding characteristics of antimicrobial peptides with PAMAM dendrimers were studied in aqueous solution at physiological pH, using fluorescence spectroscopy. The loading efficacy of antimicrobial peptides renders the PAMAM-AMP conjugates as potential candidates for controlled AMPs delivery. **Acknowledgements:** This work was supported by the Romanian Ministry of Research, Innovation and Digitization, through the National Core Program Projects No. PN 19 35 02 01/2019 and PN 19 06 02 03/2019;

Poster T2-6

Structural and kinetic characterization of expired drugs by ^{1}H NMR relaxometry and FT-IR spectroscopy

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Abstract. Expired drugs present an important problem for human health as well as for environmental protection. A large percentage of such drugs are not properly collected and destroyed after expiration and traces of active substance can be found in rivers and lakes. Therefore the problem of drugs dissolution in liquid mediums is of a great importance for water decontamination. FT-IR spectroscopy is used for the structural characterization of a series of expired drugs found as tablets, capsules and powder. The FT-IR spectra measured for expired drugs are compared with the measured spectra for non-expired drugs. For many of such drugs only small changes have been observed indicating certain integrity of the active molecule. The dynamics characterization of expired and in-term drugs was made from ^{1}H NMR relaxometry data. For that, the recorded NMR signal (at CPMG pulse sequence) was analysed by inverse Laplace transform in order to obtain the distribution of the transverse relaxation time, T_2. The expired drugs show a larger mobility compared with the in-term drugs. The solubility in liquid mediums with different pH was assessed from the kinetic measurements of i) electrical conductivity of a 200 ml solution with adjusted pH and ii) in time repetitive measurement of T_2-distribution. Finally, the expired drugs were classified as a function of their structural and dynamic stability in liquid environment.

Poster T2-7

Nanotrenches-based flexible platform for surface-enhanced Raman scattering trace level detection

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Abstract. In the recent years, applications involving ultra-low concentration detection and identification of biomolecules using surface-enhanced Raman scattering (SERS) technique migrated toward the use of 3-dimensional SERS platforms. They increase the adsorption of analyte molecules and facilitate controlled "hot spots" formation. In this work we investigate the performance of silver (Ag) coated nanotrenches arrays for SERS sensing applications. We employed Nanoimprint Lithography (NIL) technique to fabricate well-controlled periodic nanotrenches on a flexible and transparent substrate. Three Ag films with different thickness were deposited on the imprinted substrate using magnetron sputtering. Their sensitivity and detection limit were determined using crystal violet as analyte. The SERS measurements indicate that a detection limit of 10^{-8} M of crystal violet in water solution is feasible for all three Ag films making them very promising detection platforms for biomedical applications.
Acknowledgements: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-TE-2019-0910, within PNCDI III and Core-Program, Project No. PN 19 35 02 01.

Poster T2-8

^{1}H NMR relaxometry and FT-IR spectroscopy used for characterization of organo-mineral fertilizers based on biosolids

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Abstract. Biosolids from stabilized sludge presents a high fertilization potential due to its rich content of nutrients and organic matter. Three formulas of organo-mineral fertilizers based on biosolids were manufactured having at least 2 % N, 2 % P2O5, and 2 % K2O. The content of N, P and K in the final formula was measured using specific reactants combined with VIS-nearIR spectroscopy. Additionally, all three formulas were characterized by advanced 1H NMR relaxometry and FT-IR spectroscopy. Four dynamical components were identified in the T2-distribution showing that the rigid component is into a percentage larger than 90 %. In order to evaluate the release properties of organo-mineral fertilizers dynamic measurements of electric conductivity and pH were performed, by placing 0.25 g of formulas (V1, V2 and V3) in 200 ml of distillate water or acid solution. It was found that V3 present the smallest release velocity, but release the largest amount of fertilizers. Two release mechanisms were observed.

Poster T2-9

Surface-enhanced Raman spectroscopy of endosulfan pesticide on silver nanoparticle films fabricated by convective self-assembly

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Abstract. The protection of water resources has been identified as top priority by the European Commission. Pesticides are among the most hazardous chemicals, resistant to environmental degradation, requiring strict monitoring. Surface-enhanced Raman spectroscopy (SERS) is one of the most versatile analytical techniques for the detection of chemicals at ultralow concentration, due to enhancement of the otherwise weak Raman scattering of molecules by coupling to plasmonic nanostructures. Here we report our results concerning the SERS characterisation of α-endosulfan (α-ES) pesticide on the surface of colloidal silver nanoparticle (AgNPs) films prepared by convective self-assembly (CSA). The chemically synthesized AgNPs and the assembled films are characterized by Uv-Vis spectroscopy and electron microscopy. SERS measurements of α-ES on bare or functionalized AgNPs are explored and analyzed in correlation with DFT calculations. These results constitute a step towards the development of dual SERS-electrochemical sensors for detection of pesticides in surface waters.
Acknowledgements: The research leading to these results has received funding from NO Grants 2014-2021, under Project contract no. 32/2020.

Poster T2-10

Thin layer gold-based substrate for pathogens SERS detection and quorum sensing monitoring

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Abstract. Biosensing using surface-enhanced Raman scattering (SERS)-based platforms is developing towards point-of-care (PoC) solutions in more flexible, wearable, ready-to-use and affordable solid substrates. This work proposes the use of gold (Au) thin layer-based substrates for SERS sensing, in 'real-life' applications. Gold thin films with different thicknesses were deposited by magnetron sputtering technique on commercial glass slides. Their plasmonic properties were confirmed by AFM analysis which suggested that the sputtering process generates rough surfaces composed of globular clusters of a few nm ranges, smaller with respect to the wavelength of the exciting light. The analytical sensitivity of the substrates was tested by detecting bacteria in Raman and SERS effect conditions. The thickness of the Au layer was found to play a significant role in the SERS enhancement. Thus, we report on fabricating a SERS-active substrate appropriate for fast bacteria detection directly from a 3 µL droplet of sample. Ready-to-use, simple, cheap and the multi-assay capacity by using all ten microchannels for different analytes ultra-sensitive detection are key advantages of the herein proposed SERS substrates. **Acknowledgements:** This work was supported by a grant of the Romanian the Ministry of Research, Innovation and Digitization, CNCS – UEFISCDI, project number PN-III-P1-1.1-PD-2016-0475, within PNCDI III.

Poster T2-11

FT-IR spectroscopy used for identification of cancer specific biomarkers in blood plasma

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Abstract. Colorectal cancer is among the widespread malign types of digestive cancers. In this study the Fourier Transform InfraRed spectroscopy (FT-IR) method is used for the identification of specific features associated to the colorectal cancer from native and deproteinized blood plasma and from blood plasma proteins. The blood samples were collected from patients with confirmed colorectal cancer and from healthy voluntaries for comparison. The FT-IR spectra were divided into specific regions. A numeric deconvolution procedure was applied in order to quantify the integral area of peaks of interest which finally were associated with specific biomarkers of metabolites response in colorectal cancer. A statistical analysis in principal components was applied in order to identify the most important FT-IR spectral parameters for the differentiation between samples belonging to patients with colorectal cancer and healthy volunteers, and for the evaluation of the degree of method sensibility and specificity.

Poster T2-12

Molecular dynamics investigation of oligonucleotide-functionalized gold nanoparticles

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Abstract. CRISPR/Cas9 is a genome editing technique that targets and corrects unwanted gene mutations, with high-impact applications in many fields, including medicine and agriculture. The major limitation that occurs when implementing the CRISPR/Cas9 technology is the off-target activity. In order to improve the targeting efficiency, oligonucleotide-functionalized gold nanoparticles have been employed for successful delivery of CRISPR/Cas9 in vivo to repair errors in the dystrophin gene. An in-depth and comprehensive understanding of the CRISPR/Cas9-Gold-based delivery vector is crucial in improving efficiency and reducing off-target effects. In order to investigate the surface coverage of functionalized gold nanoparticles, we employed molecular dynamics simulations. The behaviour of different surface coverage densities, used for CRISPR/Cas9 delivery application, are compared. The results show that various surface densities of oligonucleotide-functionalized gold nanoparticles lead to the formation of different packing of DNA strands on the gold surface. **Acknowledgement:** This research was funded by the UEFISCDI public institution under the Romanian Ministry of Education PN-III-P1-1.1-PD-2019-0292, Contract number PD 37/2020.

Poster T2-13

Surface-enhanced Raman spectroscopy of propranolol on different SERS substrates - a step towards dual SERS-electrochemical sensors for pharmaceutical pollution monitoring

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Abstract. Pollution of water by pharmaceuticals is a general environmental problem that requires routine monitoring of pollutants. Conventional methods used to quantify pharmaceuticals are relatively expensive and generally require long analysis time associated with the difficulties to perform field analyses. In this context we focus on developing a highly accessible analytical platform for fast, selective and ultrasensitive detection of these dangerous pollutants by combining SERS and electrochemistry. Here we present our recent efforts in obtaining and analyzing SERS spectra of β-blocker propranolol on different SERS substrates including self-assembled nanoparticle films and metal-coated microsphere arrays. **Acknowledgement:** This work was supported by a grant of the Romanian Ministry of Education and Research, CCCDI-UEFISCDI, project number PN-III-P2-2.1-PED-2019-5473.

Poster T2-14

^{1}H NMR spectroscopic characterization of inclusion complex of Desferrioxamine B chelator and b-Cyclodextrin

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Abstract. In this work, the complexation between desferioxamine B (DFOB) and β-Cyclodextrin (βCD) in solution was investigated using ^{1}H NMR spectroscopy. An upfield shift of the H3 and H5 protons of β-CD, located inside the cavity, was observed when the molar ratio [DFOB]/[β-CD] increases. Similarly, some of the protons of DFOB molecule presented downfield shifts when the content of β-CD increased. Using the continuous variation method, a 1:1 stoichiometry is proposed. With this hypothesis the association constant is calculated using a nonlinear least-square regression analysis implemented in CONSTEQ, a software developed in our group, and an association constant K=251 M^{-1} is determined. A theoretical molecular docking study is additionally performed to ascertain possible conformations of the inclusion complex.

Poster T2-15

Effect of ultrasound-assisted extraction parameters on bioactive compounds from grape marc

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Abstract. The influence of the ultrasound-assisted extraction (UAE) parameters (time of 10 and 60 min and temperature of 30 and 65°C) on the total polyphenol content (TPC) and total anthocyanin content (TAC) in the hydroethanolic extracts of grape marc were investigated. It was shown that the application of ultrasound for 10 minutes, and the extraction temperature changed from 30 to 65 ° C, TPC increased by 10.6%, and in the case of TAC increased by 13.4%. In the case of applying UAE for 60 min, the extraction yield of TPC increased by 11.9% and in the case of TAC by 14.3%. It was also found that at the extraction temperature of 65°C, increase of ultrasound application time from 10 to 60 min, the TPC and TAC in the marc extracts decreased by 3.7% and by 7.6% respectively. Sensitivity analysis showed that the extraction temperature has a more essential influence on the of bioactive compounds content in the grape marc extracts than the duration of ultrasound application. **Acknowledgments**. The authors would like to thank the Project 2SOFT/1.2/83 Intelligent valorisation of agro-food industrial wastes, funded by the European Union, within the program Cross border cooperation Romania - Republic of Moldova 2014-2020.

Poster T2-16

Optimizing the extraction of pectin from apple pomace

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Abstract. In the paper analyzed the quality of pectin extracted from fresh apple pomace, from frozen and dried pomace, obtained at the Floresti juice factory. For each type of raw material, the extraction conditions (solvent volume, acid concentration, duration and temperature) were optimized to obtain a maximum yield. Unpurified pectin, extracted from fresh pomace, has a lighter color and a characteristic luster. Unpurified pectin, extracted from dried apple pomace, is brown. Pectin obtained from frozen pomace contains starch, which gives it a matte appearance. The mass fraction of extracted crude pectin varies between 14-34% DW, depending on the nature of the raw material and the extraction conditions. Fresh apple pomace is an excellent source of pectin (22-34%), the pectin obtained is more hygroscopic. Dried apple pomace is also a rich source of pectin (26-30%), for its extraction a lower volume of solvents is required. Frozen apple pomace showed a lower yield (14-18%), due to the lack of heat treatment of pomace before freezing to deactivate the enzymes responsible for pectin degradation. **Acknowledgments**. The authors would like to thank the Project 2SOFT/1.2/83 Intelligent valorisation of agro-food industrial wastes, funded by the European Union, within the program Cross border cooperation Romania - Republic of Moldova 2014-2020.

Poster T2-17

PAMAM dendrimers as a nanocarrier for Nalidixic acid delivery

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Abstract. Nalidixic acid (NAL) was the first synthetic clinically applied quinolone derivative antibiotic, used in the treatment of urinary tract infections. It is the only FDA approved quinolone drug for pediatric formulation. According to BCS, Nalidixic acid belongs to the class II drugs with high permeability and low solubility (<0.1 mg/L), insufficient to dissolve the recommended dose under normal conditions. In order to improve its bioavailability, we performed a study regarding the incorporation into different types of PAMAM-dendrimers, as delivery agent by applying freeze-drying procedure. The dendritic structures were of different generations (G4 and G5) and possessed -OH and -NH_2 terminal functional groups. The loading of NAL and supramolecular complex formation with these nanostructures was confirmed by PXRD, DSC and FTIR techniques only in the case of PAMAM-NH_2-G5. The complex stoichiometry between NAL and PAMAM-NH_2-G5 was established by ^{1}H-NMR, being 16:1. The *in vitro* release of NAL from the supramolecular complex was evaluated by UV-Vis spectroscopy using the dialysis bag method. It was observed that the release of NAL contained in the complex reached a percent of 90% compared to 54% of pure drug within 6 hours. These results sustain the improvement of NAL properties making the new supramolecular complex an interesting formulation for developing solid oral dosage form of enhanced bioavailability and therapeutic effect.

Poster T2-18

Three ways to choose between two attosecond pulses

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Abstract. Based on numerical calculations, we propose a new experimental beamline for high-order harmonic generation (HHG) of mid-infrared femtosecond laser pulses. The advantage of the proposed configuration is that it allows the generation of **two successive** (high-harmonic) attosecond pulses having separate spectral content, but both in the XUV regime. We demonstrate that the two attosecond pulses have **naturally separated** spectral content, which results from macroscopic HHG in Helium gas medium. With the proposed experimental parameters the gap between the two spectral domains is close to the onset of the water window (282–533 eV). Coherent light sources in the water window are important for the ultrafast dynamic imaging of biological samples in water medium. We propose here three scenarios: (1) with the use a low-pass spectral filter the first attosecond pulse below 300 eV is kept with its total flux; (2) with a high-pass filter the second attosecond pulse is preserved above 300 eV; (3) without filtering a double attosecond pulse emission with fixed temporal separation is obtained. The spectral separation of successive attosecond pulses is an example of space-time coupling in nonlinear optics, good candidate to be further explored and exploited both theoretically and experimentally.

Poster T2-19

3D metallic nanotrenches arrays fabricated using nanoimprint lithography

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Abstract. High-resolution nanoarrays are state-of-the-art elements frequently used due to their dependence on the optical property of size, shape and periodicity. Nanoarray architectures can be tailored to be used in the fabrication of nanodevices for electronics, photonics and biotechnology. Nanoimprint lithography (NIL) is a simple, reproducible and scalable method to create nanostructures over a large area. NIL enables the production of various periodic nanostructures on flexible substrates. Metallic nanotrenches show unique and attractive properties capable of ultrasensitive detection of molecules, active modulation as well as potential electrochemical applications. We report on a 3D plasmonic nanotrenches arrays fabricated by NIL on a flexible and transparent substrate with 300 nm height and 400 nm width, 800 nm pitch, metalized with gold (Au) and silver (Ag) with thicknesses of 25 nm, 50 nm and 100 nm using magnetron sputtering deposition technique. For uniform nanotrenches imprinted in the substrate, the NIL process parameters were optimized. The topography of 3D metallic nanotrenches was assessed from Scanning Electron Microscopy (SEM) images. **Acknowledgements:** This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-TE-2019-0910, within PNCDI III, and through the Core-Program, Project No. PN 19 35 02 01.

Poster T2-20

Environmental degradation and pigments influence on plastics waste determined by Raman Spectroscopy: sorting algorithm and plastic Raman database

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Abstract. Globally, plastic pollution became one of the most pressing environmental issues being a high concern in many research sectors. Recycling including the sorting process is an important step in transition toward circular economy. Among the challenges posed by macro- and microplastics from environment, one is to collect and sort them at feasible costs for reuse purpose. Making use of Raman Spectroscopy, we are able to sort the mix of plastic waste based on their unique spectral fingerprint. However, the characteristic plastic Raman signal can be altered on one hand due to natural factors such as long term solar atmospheric or seawater exposure, biofilm deposit or other aggressive agents and, on other hand, due to intrinsic factors such as pigments, fillers or other blends components. To date, little is known regarding their influence on the Raman spectral feature of plastic. Thus, we aimed to determine the molecular changes related to aging and pigments of a high stock of plastic degraded for years in environment. More than a Raman spectral characterisation of plastic, a sorting algorithm and a plastic Raman database were proposed to support an efficient and a proper plastic waste management based on Raman sorting technique.

Poster T2-21

Synthesis and molecular interaction of a novel diphenolic hidrazinyl-thiazole compound with strong antioxidant and antiradical activity with HSA

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Abstract. In this study we designed, synthesized and analyzed a water-soluble hybrid molecule presenting a good antioxidant and antiradical activity, namely Dihydroxy-Phenyl-Thylthiazol-Hydrazinium chloride (DPTH) which contain 2',4'-dihydroxyaceto¬phenone and the 2-hydrazinyl-4-methyl-thiazole linked through a Schiff base. This molecule presented a very good antiradical scavenging and antioxidant activity and half of the EDTA Fe(II) chelation activity in the in vitro evaluations. The main goal of this study is to quantitatively evaluate the interaction between DPTH and HSA to characterize the nature and forces underlying the formation of a molecular complex. To fulfil this goal, we analysed their interaction using ITC, NMR and molecular docking. **Acknowledgements.** This work was financially supported by Core Program, Project PN 19 35 02 01.

Poster T2-22

Mine drainage treatment using *Scenedesmus* spp., *Chlorella* spp. and *Anabaena* spp. microalgae

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Abstract. Mine drainage (MD) causes serious damage to the environment due to its high levels of metals. Thus, efficient, cost effective and eco-friendly methods need to be developed for its treatment. In the present study, the suitability of three microalgae (*Scenedesmus* spp., *Chlorella* spp. and *Anabaena* spp.) for MD treatment was investigated. The microalgae cultures were used for MD treatment when the exponential phase of growth was reached. The pH, conductivity and metals content (Cu, Zn, Fe, Ni, Cd, Mn, Pb) were determined at established time intervals during 15 days of growth. Also, the phytotoxicity effect of MD was studied on corn, beans, tomatoes, onions and mustard seeds before and after treatment with the selected species. Relative growth index, inhibition index and germination index were calculated. The results showed a high efficiency of metal removal and high reduction of toxicity after microalgae treatment. **Acknowledgment**. This work was funded by the Romanian National Core Program, project no. PN 19-18.01.01 (contract no. 18N/08.02.2019).

Poster T2-23

Potential of coltsfoot for biomonitoring metal polluted soils

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Abstract. Coltsfoot (*Tussilago farfara* L) is an invasive perennial herb adapted to neutral pH soils with low nutrient and high metal contents. Its suitability as a biomonitor of metal pollution in soils from industrial (Baia Mare) and urban (Cluj-Napoca) areas was assessed using soil to plant transfer factors (TFs) calculated as the ratio of the metal contents in coltsfoot leaves and in soil. The results showed 10-fold higher contents of Cu, Cd and Zn and 100-fold higher contents of Pb in the coltsfoot leaves grown in the industrial area, than in those grown in the urban area, while the content of Cr and Ni were comparable. The TFs were higher for Pb and Cd in industrial area, for Cu in urban area and comparable for Zn, Cr and Ni, but lower than 1 for each metal in both areas. These findings suggest that coltsfoot could be used to biomonitor metals in moderately polluted soils, as at high metal contents coltsfoot may develop an adaptation mechanism to limit the uptake of toxic metals.

Poster T2-24

Li uptake, accumulation and effect on *Salvinia natans* macrophytes metabolism

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Abstract. Lithium (Li) is a highly used element in electromobility and in other energy-storage manufacturing processes due to its excellent physical and chemical properties such as excellent conductor of heat and electricity. The use of aquatic plants for the uptake of Li from contaminated aqueous solutions and the production of Li-enriched biomass presents benefits for the circular economy. The aim of this study was to investigate the capacity of *Salvinia natans* macrophytes to uptake and accumulate Li from mono- and multielement aqueous solutions. The plants were exposed to various Li concentrations (10-50 mg/L Li as mono-, and 20 mg/L Cu, Zn, Cd and Li as multielement solution) for 7 days. The Li uptake and accumulation by the aquatic macrophytes metabolism was assessed by photosynthetic pigments, total protein contents, and antioxidant activity. The Fourier-transform infrared (FTIR) spectroscopy was performed to provide information on the plant's functional groups, after the Li treatments. The Li content in plants was determined to assess the synergistic or antagonistic interaction with the macro-and micronutrients from the growing medium. **Acknowledgment.** This work was funded by the Romanian National Core Program, project no. PN 19-18.01.01 (contract no. 18N/08.02.2019).

Poster T2-25

Metal removal from mining-impacted water by a green technology using *Salvinia natans*

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Abstract. *Salvinia natans* is a free-floating macrophyte having the ability to accumulate high amounts of metals. The objective of this study was to evaluate the impact of *Salvinia natans* on surface water quality affected by the mining activities conducted in the proximity of the water courses. Heavy metal pollution index (HPI), heavy metal evaluation index (HEI) and water quality index (WQI) were used as tools to investigate the quality of water after the phytoremediation process. *Salvinia natans* showed a good ability to remove various metals from mining-impacted waters. Removal efficiencies of 85.7%, 80.7%, 73.4% and 62.8% were obtained for Cd, As, Pb and Cu, respectively after 72h of treatment, while the WQI values improved with a maximum of 45.6% after phytoremediation. Therefore, *Salvinia natans* can be recommended as an effective biofilter to improve the surface water quality from contaminated mining areas. Acknowledgment. This work was funded by the Romanian National Core Program, project no. PN 19-18.01.01 (contract no. 18N/08.02.2019) and project "Entrepreneurial competences and excellence research in doctoral and postdoctoral programs - ANTREDOC", project co-funded by the European Social Fund.

Poster T2-26

Cold plasma processing of seeds as non-chemical, green technology for production stimulation

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Abstract. Cold plasma has been gaining a lot of attention in the past few years as an agricultural green technology being used for microorganism inactivation, stimulation of germination and growth, increasing the consumer safety in the case of processed plants or fruits, and so on. In this work we focused on the application of this technique for the processing of seeds used to produce sprouts. These have become more popular in European diets. However, there are several issues regarding their production due to the possible contamination that can pose threats to the consumer and also due to their very short shelf life. Our results show that fast green processing of the seeds can lead to the growth acceleration of the sprouts without affecting their biochemical parameters, and increase the shelf life for the sprouts obtained from plasma treated seeds.

Poster T2-27

Ultrasensitive spectroscopy of DNA from *in vitro* grown *Solanum tuberosum* L. leaves

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Abstract. Nucleic acids from *in vitro* grown *Solanum tuberosum* L. cultivars and populations were investigated at different laser lines and at several acidic pH values by surface-enhanced Raman spectroscopy. Modified SERS intensities of nucleic acids bands were observed upon lowering the pH, being a proof of binding affinity changes of DNA with silver nanoparticles and of structural changes induced at acidic pH in the DNA molecular groups. **Acknowledgements**: This work was partially funded from the Romanian Ministry of Education and Research through projects PN 19 35 02 01 (core program) and 25N/2019 BIOSERV (core program PN 2019-2022 BIODIVERS 3).

Poster T2-28

Rydberg-type electronic excited states in sodium-doped water clusters

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Abstract. Electronic transitions in sodium-doped water clusters were investigated considering the CCSD-type coupled-cluster level of theory. The equation-of-motion coupled cluster method combined with the second similarity transformation expanded on the domain based local pair natural orbitals (DLPNO-STEOM-CCSD) provides an efficient way to calculate excitation energies of the Rydberg-type electronic transitions with high accuracy. The results for different electronic transitions show Rydberg-type orbitals with different special configuration, indicating large delocalization over the water molecules for the $3s^1$ electron of the sodium atom.

Poster T2-29

Melittin: a new use in cancer therapy

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Abstract. Antimicrobial peptides are a class of molecules synthetized by a variety of organisms as innate defensive means against different pathogens. These natural compounds have been also identified as a promising alternative to widely used drugs against infections and cancer cells. Considering their action mechanism, antimicrobial peptides can be viewed as future chemotherapeutic alternatives, with the advantage of low propensity to drug resistance. In this study, we evaluated the efficiency of an antimicrobial peptide, Mellitin (Mel) along with proton irradiation (2 and 6 Gy), against spheroids formed from two cell lines: HT-29 (human adenocarcinoma/colorectal cell line) and HCT-116 (human carcinoma/colorectal cell line). Spheroids' evolution, cell viability, their ATP levels and LDH release were monitored at 24h and 48h timepoints after the applied treatment. The results show a significant drop in cell viability and cellular ATP level, for all the experimental conditions. The simultaneous use of the two types of treatment (Mel and proton irradiation) has a synergistic effect against the spheroids. **Acknowledgements**: This work was supported by the Romanian Ministry of Research, Innovation and Digitization, through the National Core Program No. PN 19 06 02 03/2019.

Poster T2-30

Materials based on lanthanide complexes with polycarboxylic acids - synthesis, spectroscopic characterization and magnetic properties

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Abstract. Synthesis of new polyhomonuclear or polyheteronuclear lanthanide coordination complexes of some lanthanoids with polycarboxylic acids are described. The influence of the pH and molar ratio ligand:lanthanide on the composition of the complex was investigated. Spectroscopic characterization of all new compounds by appropriate means (IR, UV-VIS, NMR, single crystal or powder X-ray diffraction, powder neutron diffraction etc.), magnetic measurements and their correlation with molecular structure are presented. **Acknowledgments:** This work was carried out in the framework of Romanian-JINR cooperation (No. 39, Order 365/11.05.2021)

Poster T2-31

Synthesis, physicochemical properties, crystal molecular structure and DFT investigation of an organobismuth(III) bis(dimethyldithiocarbamate)

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Abstract. Two new organobismuth(III) dimethyldithiocarbamate, i.e. [2-(Me2NCH2)C6H4]Bi(Cl)(S2CNMe2) (4) and [2-(Me2NCH2)C6H4]Bi(S2CNMe2)2 (5) derivates were obtained starting from [2-(Me2NCH2)C6H4]BiCl2 (3) and sodium dimethyldithiocarbamate in 1:1 and 1:2 molar ratios. Compounds 4 and 5 were fully characterized by spectroscopic methods. The molecular structure of the organolithium derivate [2-(Me2NCH2)C6H4]Li (1) used for the synthesis of organobismuth(III) precursors was determined at 150 K and found to be very similar to that measured at room temperature, previously reported almost 40 years ago. For compound 5 the solid-state molecular structure was also determined by single crystal X-ray diffraction. A DFT, NBO and Hirshfeld surface analysis was carried out for compounds 1 and 5 in order to establish the profile and energy of frontier orbitals, the nature of intra- and intermolecular bonding interactions and the results were compared with those observed experimentally in the structures determined by X-ray diffraction. **Acknowledgments:** This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE-2020-2651, within PNCDI III.

Poster T2-32

Separation and characterization of specific anti-dicamba antibodies using antigen type SiO_2-based nano-immunosorbents

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Abstract. Interaction between antigens and antibodies *in vitro* is used to detect either the antigen or the antibody by the ELISA technique. The need for the purification of specific antibodies is given both by the source from which they are isolated and by their subsequent use. The aim of separating anti-dicamba antibodies is to select from the polyclonal antiserum the specific antibodies with the highest affinity anti-dicamba antibodies. Functionalization of nanoparticles with antigens combines the properties of the silica nanoparticles with the specific and selective recognition ability of the antibody-antigen interactions. Nano-immunosorbents based on silica nanoparticles functionalized with dicamba (3,6-dichloro-2-methoxybenzoic acid) antigen were developed to be used for separation of specific anti-dicamba antibodies from rabbit serum.

Poster T2-33

Compressing VQE circuit with applications in the study of small molecules

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Abstract. Quantum computers allow us to efficiently solve problems that would normally be intractable for classical hardware. An example of such a problem would be determining the minimum eigen value of an operator. Although technology is in continuous development, right now the dimensions of a real QPUs are small and quantum computing simulators are limited. In this study, we tested various methods of optimizing the dimensions of such a circuit in order to reduce the number of qubits as well as the number of gates. The results show a dependence between optimization time and circuit dimensions. So, we can say now in which situations the optimization step is useful or redundant.

Poster T2-34

New non-contact photopyroelectric method for thermal diffusivity investigation of porous solids: theoretical approach and mathematical simulations

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Abstract. A new photopyroelectric (PPE) method, suitable for the direct measurement of the thermal diffusivity of porous solids is proposed. The technique makes use of a very simple detection cell, composed by only three layers: a transparent pyroelectric sensor and an opaque sample (porous solid), separated by a layer of air (coupling fluid). The methodology is based on two successive frequency scans of the PPE signal, one in front and one in back detection configuration, followed by a self-normalization of the two runs. In the paper, the theory of both back and front configurations is developed, considering as heat propagation mechanisms the heat propagation by conduction and also the heat losses by convection. The phase of the normalized signal is used as a source of information. The sample's thermal diffusivity is finally obtained via a multiparametric fit with three fitting parameters: the sample's thermal diffusivity, the thickness of air gap between sample and sensor, and the heat losses by convection at the irradiated sample's surface in back configuration. Mathematical simulations are used in order to analyse the influence of each fitting parameter on the results.

Poster T2-35

Crystallization process development of Febuxostat most stable polymorph and of a soluble salt thereof

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Abstract. Febuxostat (FB) is an active pharmaceutical ingredient (API), poorly water-soluble and therefore poorly bioavailable. FB is used for the treatment of hyperuricemia in gout, as inhibitor of xanthine oxidase, to reduce uric acid production. With the aim of improving the aqueous solubility, we investigated the crystallization process of the FB tromethamine salt (Tro1). In addition, we were able to grow crystals of the most stable polymorph of FB, designated as form A in the literature. Crystallization process development of the Tro1 and form A was performed in a controlled manner using the Crystal 16™. The crystallization process parameters were established by determining the Meta-stable Zone Width (MSZW) while performing two thermal cycles in a suitable solvent system (2-ethoxyethanol) using a broad temperature range (5 - 90°C) and different concentrations. The formation of Tro1 and form A was evidenced by X-ray powder diffraction. We can conclude that Tro1 can be reliably crystallized in 2-ethoxyethanol by using high starting concentrations (> 200 mg/mL). Furthermore, crystals of form A were successfully grown in the same solvent at concentrations above 100 mg/ml. Crystal structure determination of form A will be attempted in a future work. **Acknowledgement:** We would like to thank Technobis Crystallization Systems BV for training on the Crystal 16™ device.

Poster T2-36

Effects of propolis extracts on model membranes

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Abstract. The most complex product that can be obtained from beekeeping (*Apis mellifera*) is propolis. Propolis is produced by bees by mixing resins collected from plants, especially trees, with wax and various substances secreted by them (e.g., substances secreted by their salivary glands). Its chemical composition depends on the geographical area, the local flora and the climatic zone. In this paper, we evaluated the effects produced by hydroalcoholic extracts of propolis, obtained from samples collected from different geographical regions of the country, using fluorescence spectroscopy, on two types of model lipid membranes, which mimic the membrane of mammalian and bacterial cells, respectively. The effects on membranes were correlated with the amounts of the main phenolic components in the propolis samples (flavones and flavonols, flavanones and dihydroflavonols and the total phenol content), determined using UV-VIS spectroscopy. **Acknowledgements:** This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-PD-2019-0778, within PNCDI III, and through the National Core Program No. PN 19 06 02 03/2019.

Section T3:

Energy Efficiency and High-Tech Engineering

Oral T3-1

Advances of electromagnetic energy harvesting through antenna-metamaterial coupling

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Abstract. The proposed goal in this research topic is to increase the efficiency to capture and convert the electromagnetic waves from the GSM (860 - 950 MHz) and WLAN frequency bands (2.4 - 2.5 GHz), by using a resonant coupling between a rectifier antenna and a metamaterial. For the design of the metamaterial resonator, a microstrip configuration is chosen in the form of a logarithmic copper spiral. The characterization of the antenna-metamaterial assembly is performed with the Agilent PNA-L Vector Network Analyzer, N5230A (10 MHz - 40 GHz), in a emission-reflection measurement type mounting, for a pair of identical metamaterial-antennas placed face to face at a fixed distance. For the frequency range 500 MHz to 4 GHz, the range of interest for common applications, it is observed that the metamaterial-antenna coupling produces at least a doubling of the antenna gain.

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Oral T3-2

Analysis of Demonstration and Characteristic for the ±35kV MVDC

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Abstract. In the future, it is expected that the application of DC systems will gradually increase due to the increase in new&renewable energy, DC load and distributed power. In this paper, we demonstrate ±35kV MVDC for the new&renewable energy and distributed power. At this time, compared to the existing AC line, we intend to establish the MVDC-class transmission capacity standard, secure a track record, and discover a business model.

Oral T3-3

Structural Safety Analysis of 200 kW Class Wind Turbine Nacelle Cover for Islands

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Abstract. Remote islands, off-grid to the mainland, rely on diesel generation for own electricity supply. In order to decrease carbon gas production, diesel generation should be minimized and renewable energy applications such as wind energy and solar energy should be expanded. In this study, a nacelle cover for a 200 kW wind power generator for an energy independent island was designed and its structural safety was analyzed. Stress, deformation and buckling were analyzed for each load case according to the GL Guidelines. As a result, the maximum deformation was 12.99 mm by rear wind (load case 4), the maximum von Mises stress was 96.89 MPa by left wind (load case 3) and the safety factor was more than 2.58 in all load cases. In addition, the critical buckling strength value (safety factor) was 2.04 for the lowest value in rear wind (load case 4). The structural safety of the nacelle cover design was confirmed.

Oral T3-4

Case Studies for Non-Detection of Islanding by Grid-Connected In-Parallel Photovoltaic and Electrical Energy Storage Systems Inverters

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Abstract. In Korea, there was a rule for Renewable Energy Certification with weighting 5.0, to expand grid linkage capacity and to improve the stability of the grid to accommodate photovoltaic (PV) systems in a distributed power system. Due to this rule, many power companies and operators are trying to install electrical energy storage systems that are able to operate in conjunction with PV system power. These systems operate in parallel at the same grid connection point. This paper presents the results of case studies on the failure to detect islanding operation. Test evaluation devices that could be bi-directionally charged and discharged were implemented for an islanding detection test. Testing was conducted under a variety of operating conditions. When a single inverter was operated under the islanding condition, it was stably stopped within 0.5 s using the Korean grid-code standard. However, when two inverters were operated at the same time under the islanding condition, islanding detection failed and the two inverters continued to feed the connected RLC (resistor, inductor, capacitor)oads in the isolated section known as an island. Different algorithms used by PCS (power conversion system) manufacturers to detect islanding might cause this phenomenon. Therefore, it is necessary for a new PCS test standard to detect islanding.

Oral T3-5

Tuning of the Magnetocaloric Effect in the $Dy(Fe_{1-x}Cu_x)_2$ System

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Abstract. Magnetic refrigeration based on the magnetocaloric effect (MCE) is a promising alternative to the vapor compression cycle, being more energy-efficient and environmentally friendly. The performance of the magnetic refrigerator is determined by the MCE material, which should have a high magnetization and a Curie temperature close to 300 K for room temperature applications. One class of suitable MCE materials is the $Dy(Fe_{1-x}Cu_x)_2$ system. These materials have highly tunable Curie temperatures and a high magnetic moment carried by the rare earth, which generates large MCE values. The $Dy(Fe_{1-x}Cu_x)_2$ **s**amples with $0 \leq x \leq 0.5$ were prepared by arc-melting the constituent elements under Ar atmosphere. The compounds are single phase and crystallize in the $MgCu_2$-type crystal structure, the lattice parameters showing a slight increase with Cu content. All of the samples show ferrimagnetic order. As the Cu concentration increases, the Curie temperatures decrease, however, the saturation magnetization values increase. Electronic structure calculations using the PAW+U method were performed in order to support the experimental observations, showing a good agreement between theory and experiment. The magnetocaloric effect was evaluated for each sample from magnetization isotherms measured around the Curie temperature. We discuss the potential application of these materials in magnetic refrigeration devices.

Oral T3-6

The influence of solvent on the electronic structure and redox properties of sulfonamides

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Abstract. The conjugated sulfonamides were recently proposed as a new class of redox-active materials with potential applications in battery industry. While their properties were clearly demonstrated, the influence of solvent effects upon the redox properties is not yet fully understood. We present a comparison of DFT results for electronic structures obtained for six conjugated sulphonamides in vacuum and solvent and point out the differences between them as well as the physical causes for these differences. We use these conclusions to point out to the potential applications and further research path to be followed in the quest for improve redox systems based on organic molecules. **Acknowledgements.** This research is supported by UEFISCDI Romania through the project PN-III-P4-ID-PCE-2020-0824, PCE 22/04.02.2021.

Oral T3-7

ITIM contribution to the development of a new particle detector read-out system

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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.

Oral T3-8

High temperature receiver for concentrated solar power

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Abstract. Solar power, one of the most important renewable energy sources, can be converted directly into electrical power through photovoltaic panels or it can be concentrated through optical devices and then converted into thermal and electrical power using thermo-energetic machines. The thermal receiver placed in the focal point of an optical device, like Fresnel lens, need to be compact to reduce the surface heat losses but also it needs to withstand high temperatures. In this study we present a compact design of hight temperature thermal receiver. We studied through experimental and CFD simulations the amount of concentrated solar power captured and transferred to a thermal agent, the energy losses and estimate its efficiency in different experimental conditions.

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Oral T3-9

NIR imagistic and spectroscopic investigation of ITO thin films: A non-invasive and non-destructive approach

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Abstract. The aim of our study was to investigate spectroscopic and imagistic some ITO films, deposited from suspensions on flexible polymeric substrates, in a non-invasive and non-destructive approach using NIR radiation. The deposition of the ITO particles could be done almost instantly on the entire surface due to the substrate's efficient activation. The samples investigation by NIR spectroscopy in reflection indicated a low aggregation tendency of ITO particles in the obtained thin films, while optical coherent tomography (OCT) images displayed the thickness of the substrate, as well as a good adhesion and relative uniform distribution of the ITO particles on the substrate. The contrast of the OCT images is faded, so their quality should be improved to reveal details which are not well distinguishable in the original OCT images. For this reason, the enhancement of the OCT images quality is performed by employing an image processing algorithm which consists of several steps: image sharpening, homomorphic filter, noise reduction and contrast enhancement. Demonstrative images showing the original OCT images and OCT images having enhanced visibility are illustrated. **Acknowledgements**: This work was funded from the Romanian Ministry of Research, Innovation and Digitization through Core Program, project PN 19 35 02 01.

Poster T3-1

Researches about the recycling of mobile phone

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Abstract. The lithium recycling from spent mobile phone batteries requires the integration an eco-innovative technology with reduced costs and the energy efficiency. In this paper, the active mass from a spent mobile telephone (notated with BT) will be recycled by the incorporate in the sodium diacide phosphate. The samples having the xBT·(100-x) NaH_2PO_4 composition where x = 0 – 30 weight % BT using as raw materials the black powder recovered from the disassembled telephone battery and sodium diacide phosphate were prepared by melt-quenching method. New obtained materials will be characterized by the analysis of X-ray diffraction (XRD), Infrared (IR), UltraViolet-Visible (UV-Vis) and Electronic Spin Resonance (RES) spectroscopy. The electrochemical properties as new electrode material for the applications in the lithium-ion batteries will be tested by measurements of Cyclic Voltammetry (CV). Our results obtained from varied techniques show the presence of Li_2NiO_2 crystalline phase which is responsible of electrochemical performances of the electrode materials.

Poster T3-2

Investigations on the magnetic properties of the $RFe_{11}Ti$ (R = Y, Gd and Pr) by Zr, Co and C doping

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Abstract. We present theoretical and experimental investigations on the electronic and magnetic properties of the $RFe_{11-x}Co_xTiC$ and $R_yZr_{1-y}Fe_{11}Ti$ and (R = Y, Gd and Pr; y = 0 - 0.2; x = 0 - 3) alloys. The theoretical calculations describe the dependence of the magnetic properties (magnetic moments, magneto-crystalline anisotropy energy MAE, exchange-coupling parameters) on the R/Zr and Fe/Co ratios. The Zr for R substitution in $Y_yZr_{1-y}Fe_{11}Ti$ (y = 0 - 0.2) increases the calculated total magnetic moment by increasing Zr content x but the magneto-crystalline anisotropy energy shows a slight decrease. On the other hand, the improvement of the magnetic properties (total magnetic moment and MAE) for permanent magnets applications of $RFe_{11}Ti$ based alloys appears to be efficient upon partial Co for Fe substitution. The experimental measurements are in progress to test the theoretical findings. The investigations performed within this study are focused on obtaining rare-earth free permanent magnets with enhanced magneto-crystalline anisotropy (MAE) and higher magnetization.

Poster T3-3

Influence of hydrogen adding in the Stirling engine combustion process

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Abstract. Due to the rising interest in the optimisation of the Stirling engine and the use of hydrogen as green energy, this work considers a simulated design of a Stirling engine combustion chamber and presents the effect of hydrogen adding in the Stirling engine combustion process. The CFD simulations are performed in ANSYS Fluent, in order to obtain the thermal parameters, such as the heater temperature distribution, heat flux transferred to the heater, the energy loss of the burning cavity, the temperature distribution inside the chamber as well as the ejected stream heat. The simulations were performed for concentrations of up to 10 % of hydrogen in methane. **Acknowledgment:** This paper was financially supported from the MCID, Nucleu-Program, project nr.PN 19 35 01 01.

Poster T3-4

Minimum ac impedance determination in commercial Li-ion batteries by experimental measurements

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Abstract. Healthy Li-Ion accumulators present low AC impedance or DC internal resistance. These two parameters are increasing during charging-discharging cycles until the accumulator becomes unusable. Three types of new Li-Ion 18650 accumulators with different rated capacities have been tested using galvanostatic electrochemical impedance spectroscopy. The measurements were set on Biologic VSP potentiostat device. Accumulators were charged up to 2000mAh and then ac impedance in 1Hz-10KHz range was measured. A comparative plot has been highlighting the optimum frequency (1.3-1.5KHz) corresponding to the minimum AC impedance (0.08-0.14 Ω). As the battery was aged the AC impedance has started to grow. Higher voltage discharging curve have been obtained in switching mode discharge compared with continuous discharge. This result indicates a method to supply sensitive electronic devices to voltage drop for longer accumulator usage. **Acknowledgements**: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN 19 35 01 01.

Poster T3-5

DFT investigations of early stages of formation of aluminium oxide at Al surface

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Abstract. We use the DFT and Verlet molecular dynamics to investigate the formation of aluminium oxide at the surface of Al. The model corresponds to the early stage formation of oxide; we monitor the evolution at temperatures close to RT for one or two oxygen atoms placed on top of the Al surface. The quantitative stability of the system is evaluated by calculating the free energy of the system as a function of the number of oxygen atoms and/or the type of Al surface. Out of this analysis we pin down the parameters that can favour the formation of oxide as a function of surface type as well as function of temperature. **Acknowledgements.** This research is supported by UEFISCDI Romania through the project Quantum Computation with Schrödinger cat states, contract ERANET-QUANTERA-QuCos 120/16.09.2019.

Poster T3-6

Testing a proton-exchange membrane fuel cells for an electric vehicle mobile charging station

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Abstract. Currently, in the transport sector, the technology of electric or hybrid plugin vehicles is in a continuous expansion, resulting the need to develop the infrastructure of fixed and mobile charging stations. A mobile charging station was realized during the project SmiLE-EV, composed of PEMFC, H_2 tank and batteries. Paper deals with the test results of the PEMFC (study of the behavior of the fuel cells in transient operating regimes, repeated start-stop cycles) used in this mobile charging station from on road electric vehicle supplying.

Poster T3-7

Manganese oxide – antimony oxide – lead – lead dioxide vitroceramics

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Abstract. The number of spent batteries was increased significantly in recent years along with the use of mobile phones, vehicles, and other high-tech products. In this work the vitroceramics in the $5MnO_2 \cdot xSb_2O_3 \cdot (95-x)[9Pb \cdot PbO_2]$ composition where x = 0 – 40 mole% Sb_2O_3 were synthesized by melt – quenching method using as raw materials the spent plates of a car battery (the anode as Pb source and cathode as PbO_2 source), MnO_2 and Sb_2O_3 powders. The prepared samples were characterized by XRD, IR and UV-Vis data. The electrochemical performances of the antimony – manganese - lead materials used as working electrode at a car battery were demonstrated by measurements of cyclic voltammetry. The combined results from varied techniques show that antimony ions play the important role in the conductive and electrochemical properties. **Acknowledgments:** This paper was supported by the Ro-Dubna projects, Protocol No. 53 / 2021.

Poster T3-8

Design of a semiconductor thin-film thermocouple fabricated by pulsed laser deposition

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Abstract. Silicon is one of the most used substrates for the deposition of thermoelectric materials as thin films. In this work, we report the design of a thermocouple based on thin films (in this case a pair of semiconducting copper-based chalcogenides, but it works for any kind of thin films) fabricated by pulsed laser deposition (PLD) on silicon wafers. Taking into consideration that charge transport is enhanced in the direction parallel to the surface of the film, two gold electrodes were deposited by sputtering on each thin film, the rest of the film being protected by kapton tape (for electrical and thermal insulation, and increased mechanical resistance). Upon applying a conductive paste between the gold electrodes from each film, a thermocouple is formed. An extra gold electrode applied on kapton tape is used as inter-connect between two thermocouples. A thermal insulator layer can be applied between the thermocouples, in order to maintain the thermal gradient between the two sides. The idea is to be able to connect multiple such pairs in line, in order to fabricate a miniaturized thermoelectric device.

Poster T3-9

Lead Bismuth Eutectic (LBE) as thermal agent in concentrated solar power applications

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Abstract. Heavy liquid metals offer a wide range of uses in energy conversion systems due to their excellent thermal properties. Furthermore, the neutronic characteristics of different liquid metals make them appealing for fusion as well as Generation IV nuclear reactors. Concentrated solar power (CSP) systems, which can reach temperatures up to 800 °C, have recently gained popularity. Lead Bismuth Eutectic (LBE), 44.5 wt% Pb + 55.5 wt% Bi, is one of the main candidates for solar thermal applications as liquid-metal coolant, due to its physical qualities such as high thermal conductivity, low melting point (~124 °C) as well as high boiling point and low thermal expansion. The process for synthesizing the LBE alloy by induction melting, as well as the structural properties and stoichiometry analysis of LBE, are presented. The structural properties were studied by X-ray diffraction, Scanning Electronic Microscopy (SEM), Energy Dispersive Spectroscopy (EDS) and Differential scanning calorimetry (DSC).

Poster T3-10

Component identification of liquid mixtures by using computational models

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Abstract. Our experience in detecting complex biological samples such as microorganisms in biofluids by means of vibrational (Raman and Surface-enhanced Raman scattering - SERS) spectroscopies generated the need of component identification for such samples. The complexity involved in deciphering the information from the vibrational spectra lays in how many biological components and/or their derivatives are combined in the investigated biomass or specific byproducts. The complementarity of the Raman and IR fingerprints assigned to common biochemical species found mixed in different ratios as composing complex samples was explored. Herein, we are looking to identify individual components present in liquid samples by creating an *in silico* model. A robust algorithm was developed and tested on the vibrational response of two different classes: mixtures of (i) solvents and (ii) antibiotics. **Acknowledgements**: A.M.R.G. would like to acknowledge the financial support through the Core Program, Project No. PN 19 35 02 01. This work was also supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-PD-2016-0475, within PNCDI III (N. E: D).

Poster T3-11

Developing a platform to support urban energy monitoring and the co-creation of the city's energy transition

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Abstract The Cluj-Napoca Pilot within the REFLOW project focuses on the co-design of the city's energy transition and testing innovative tools in this regard. The vision of REFLOW is to develop circular and regenerative cities through the re-localisation of production and the reconfiguration of material flows at different scales. The Pilot will invest in energy efficiency, optimizing consumption,sharing open data and uniting local administrators, communities and energy service providers. The objective is to fast-track the adoption of low carbon tech within Cluj-Napoca's local context. The Pilot will conduct energy consumption analyses of one municipality-owned buildings after a retrofit kit is installed. The data will present the decrease in energy consumption. The aim is to observe the impact and the potential of circular economy-like actions for Cluj-Napoca energy efficiency practices as well as to study the synergetic positive effects of collaboration among multiple stakeholders in the community (ie public authorities, research institutes, clusters and the general public). **Acknowledgements**:This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement number 820937.

Poster T3-12

Calcium oxide - lead – lead dioxide vitroceramics

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Abstract. Today the number of automobiles is increased and the need of lead acid batteries is highly. The improvements in the recycling of car batteries must to imply the elimination of disadvantages related to the traditional recycling methods. The purpose of this work is: i) to recycle the spent plates from a car battery with high wear by an eco-innovative method; ii) to characterize of prepared materials and to test of their electrochemical performances for the applications as new electrode for the car batteries. The prepared samples were investigated by XRD, IR, UV-Vis data and measurements of cyclic voltammetry. Our results show that by the adding of calcium ions, no emissions of sulphur oxides into the atmosphere were produced. **Acknowledgments:** This paper was supported by the Ro-Dubna projects, Protocol No. 53 / 2021.

Poster T3-13

Testing and certification of front-end electronics for particle detectors

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Abstract. The front-end electronics of particle detectors are working in radiation environments, for long periods without the possibility of maintenance. That's why must be intensively tested in harsh operating conditions to guarantee the reliability and linearity on long-term. The paper presents the test methods for the certification of active dividers for photomultiplier tubes, produced by INCDTIM, as collaborating institute, for the Phase II Upgrade of Tile calorimeter of ATLAS Experiment at CERN LHC. Are described the burn-in set-up for annealing of the active dividers, the automated test bench for functional tests of ten active dividers simultaneously, and the test results for pre-production lot dividers.

Poster T3-14

An energy measurement system for battery powered applications

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Abstract. Recent development of devices and methods for energy storage and harvesting has opened a plethora of pathways towards more energy independent systems. Some applications aim for remotely operated systems, hence required to be energy independent. Therefore, for energy independent prototype systems, the measurement and counting of the internal energy flow is of great importance. An energy measurement system, developed for battery powered prototypes is presented herein. The measurement system is meant to precisely assess the values of the energy in low voltage prototypes. For this purpose it is aimed for current and voltage measurements, hence returning data that can be further processed, in order to determine the value of energy flown into the prototype. An application for energy measurement of a commercially available battery is presented herein. **Acknowledgements:** The presented work has been carried out through the Core-Program, developed with the support of the Ministerul Cercetării, Inovării şi Digitalizării (MCID), project no. PN19 35 02 03.

Poster T3-15

Optimization of river flow capture at micro-hydro power plant intake to increase electricity production

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Abstract. Depending on their location, micro-hydro power plants have various types of intakes. The goal of this research is to improve the efficiency of micro-hydropower plants that have incorporated winter inlets. Based on analysis of on-site measurements results and numerical simulations for the process of river flow capture for micro-hydropower plants, we identified a technical solution that, once implemented, can increase the electricity production capacity of the power plant, and in the same time also fully respecting the environmental requirements imposed by the authorities. The case study was realized at MHC Valea Draganului, which have a Tyrolean intake type equipped with winter intake. The installed capacity of micro-hydro power plant is 2.101 MWh, and use a Francis turbine. **Acknowledgment**: This paper was financially supported from the MCID, Nucleu-Program, project nr.PN 19 35 01 01.

Poster T3-16

Recycled and antimony-doped lead materials: XRD, SANS and voltammetric study

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Abstract. In the last ten years the production of lead grills from automotive batteries has been replaced by lead alloys with other metals such as antimony. This work describes antimony-lead materials that contain a substantial amount of 10 mol% Sb_2O_3 and varied mass compositions between Pb : PbO_2. The sources of PbO_2 (cathodic electrode) and Pb (anodic electrode) come from spent plates of a car battery. The recycled and antimony-doped materials were characterized by the analysis of X-ray diffraction and Small Angle Neutron Scattering (SANS) data. The electrochemical performances of the antimony-lead materials used as working electrode at a battery were demonstrated by measurements of cyclic voltammetry. **Acknowledgments:** This paper was supported by the Ro-Dubna projects, Protocol No. 56 / 2021.

Poster T3-17

Noises and vibrations in Cluj-Napoca

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Abstract. Noise and vibration measurements were carried out in Cluj-Napoca, in order to create a database on the potential for energy recovery in Cluj-Napoca, but also to find solutions to combat noise pollution in the city. A total of 27 measurements were performed in the areas of interest throughout the Cluj-Napoca municipality. Of interest for this study are areas with high noise, in order to estimate the level of noise and vibration. Thus, the measurements were performed in key areas for local road infrastructure, such as intersections, bridges, roads with heavy road traffic. Also of interest are the locations specific to the railway infrastructure and a series of measurements have been made in locations such as the railway station, bridges over the railway and bridges for rail traffic. These data will be the basis for making noise maps. The noise map aims to highlight the areas in Cluj-Napoca, where the noise level rises above certain limits imposed by law and thus is used to develop action plans to protect residents against exposure and reduce noise levels. At the same time, the development of energy recovery systems from noise and vibration will contribute to the transformation of noise pollution into green energy and will lead to an increase in the quality of life in the municipality. The results can be used to produce a device for converting vibrations and noise into energy, a device that can be located in noisy areas of urban areas in particular or in places with high vibrations such as factories, airports, schools, and stadiums.

Poster T3-18

Maintenance and efficiency monitoring of photovoltaic systems

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Abstract. Present study shows a multitude of internal and external parameters that affect the electricity production of a photovoltaic system. The energy production of the panels is influenced by several factors, such as the weather conditions, the positioning, the shading, the dust and the aging. To have an efficient system, maintenance is very important. This photovoltaic system is located within I.N.C.D.T.I.M. Cluj-Napoca, on the roof of the CETATEA building. It was financed by the Sectoral Operational Program " Increasing economic competitiveness ", Investments for your future and co-financed by the European Regional Development Fund. **Acknowledgment:** This paper was financially supported from the MCID, Nucleu-Program, project nr.PN 19 35 01 01.

Poster T3-19

Advanced in automated control of dynamic laser scanning of surfaces in flying spot thermography

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Abstract. The purpose of this work is to develop different non-destructive testing methods of defect detection and characterization purposes by automated dynamic infrared detection. More exactly, for quality control in airspace inspection, IR lock-in thermography coupled with flying spot thermography (laser scanning of the surface to be investigated) has been proposed. The surface scanning algorithm involved the introduction of a electrical and optical calibration procedure for the entire mechanical assembly of galvo-mirrors, along with the correct positioning of the IR camera. During the adjustments, the aim was to correlate the image obtained from the FLIR camera with the interactive movement of the coordinates of the reference points.The automatic laser scanning algorithm together with the horizontal (Ox) and vertical (Oy) laser return path on the investigated surface was performed in LabView software. After entering the operational parameters, the system calculates the number of samples required for the x coordinate, respectively the number of resulting laser scan lines. During the preliminary tests, an optimal scan time of a line was selected at 10 seconds, achieving a total of 17 scan lines at a mirror sampling rate of 100Hz. The displacement of the heat source on the surface is going to be further synchronized with the capture of the IR images by using the lock-in detection module embedded in Infrared camera and the camera trigger.

Poster T3-20

Calibration of RF matrix array detectors for environmental electromagnetic field

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Abstract. Integrated logarithmic RF detectors provide a well known solution for RF to DC conversion. The main issue of these detectors is caused by the variable output offset voltage measured in the absence of the input signal and a variable RF/DC characteristic. Thus, different RF detectors will provide slight different output signal for the same RF input. We designed and manufactured a matrix of 64 RF intelligent detectors. Each detector input is connected with a miniature antenna. Each detector output is connected with the AD input of a node microcontroller. Each node microcontroller displays data as an RGB colour and sent it to a supervisor microcontroller using a blocking asynchronous communication scheme. The supervisor is able to load at once all the 64 nodes with data. We applied a proprietary algorithm for logarithmic detectors offset and full scale reading. Based on measured data, true gain is computed by the supervisor microcontroller and sent back to the nodes. After applying the calibration algorithm, the RF matrix is able to detect the RF signal within ±2dB inhomogeneity. **Acknowledgements**: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number **PED-2019-1453**, within PNCDI III

Poster T3-21

Enhancement of SEM images quality

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Abstract. The presented work is devoted to increasing the quality of SEM images recorded on chitosan-based films containing gold nano/microentities of different sizes and shapes. Due to the differences in height and distribution of the embedded gold particles, the surface of the SEM image is not linearly illuminated and some of their edges are not clearly delimited. Therefore, a five-steps image enhancement algorithm, which increases the visibility of details content in SEM images, is developed. The proposed algorithm consists of the following imaging filters: image sharpening, homomorphic filter, anisotropic filter, contrast stretch and linearization. The benefits of applying this algorithm are illustrated by a set of demonstrative images consisting of the original SEM images and enhanced clarity SEM images as well. **Acknowledgements**: This work was funded from the Romanian Ministry of Research, Innovation and Digitization through Core Program, project PN 19 35 02 01.

Poster T3-22

Numerical model for femtosecond pulse propagation in hollow core fibers

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Abstract. High order harmonics generation by interaction of femtosecond pulses with gas media plays an essential role in obtaining attosecond pulses in the XUV or soft X-ray region. One way to increase the well-known low generation efficiency is to place the gas medium in a hollow waveguide which maintains the driving field intensity by preventing the plasma defocusing and, in the same time, ensures a long generating medium.In modeling this process one has to solve first the problem of pulse propagation in the hollow core waveguide which experimentally is fabricated by laser micromachining**.** The numerical model used to obtain field configuration along and across the waveguide was developed starting from a split step method in an arbitrary ges density profile. The way to solve the critical points of this development will be described and the behaviour of the pulse in various conditions of gas pressure, ionization levels, initial beam radial profile and pulse intensity will be presented.

Poster T3-23

Reconstruction of ultrashort laser pulses by convolutional neural networks

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Abstract. The creation and reconstruction of ultrashort (femtosecond or attosecond) laser pulses is an important field of basic research. However, a large range of applications also use such pulses (femtochemistry or ultrafast imaging for example), but all are based on physical processes, which cannot be resolved in space or time using other means of investigation. Since these pulses cannot be measured by conventional electronics, their characterization involves a special technique, called FROG (frequency resolved optical gating), which uses the pulse and a delayed copy of itself to create a spectrogram. The reconstruction method means the recovery of the amplitude and phase of the pulse from the FROG spectrogram. Here, inspired by recent studies, we propose employing a CNN (convolutional neural network) to recover the amplitude and phase of ultrashort pulses. The input to the CNN is a set of FROG traces (computer simulated or experimental), which is trained by comparing the recovered pulses to known pulses. The method will provide a faster way to recover ultrashort pulses, and to avoid using conventional recovery algorithms like PCGPA (principal component general projections algorithm) for example.

Poster T3-24

Structural Evolution and Physical, Optical and Electrochemical Properties of Manganese Ions in Lead Glass

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Abstract. Lead glass-ceramics containing transition metal ions are of huge interest because of their electrical and optical properties that makes them suitable for many applications such as electrochemical, electronic, and electro-optic devices. The manganese ion is a highly fascinating ion among different transition metal ions do to the multiple valence states Mn^{2+}, Mn^{3+} and Mn^{4+}. Their simultaneously presence in glass depends on the quantitative properties of glass formers and size of the ions in the glass structure and influence on several physical properties of the host glass. In the present study, lead-manganese glass ceramic, obtained by melt quenching technique was investigated both as alternatives to rare-earth doped luminescent materials and as new electrode materials for lead-acid battery. Characterization techniques including XRD, FTIR, UV-Vis, PL, EPR spectroscopy and Cyclic Voltammetry were used to analyze the compositional dependence of the structural, optical, and electrochemical properties of lead-manganese glass ceramics. **Acknowledgments**: This paper was financially supported by the Ministry of Research, Innovation and Digitization: Nucleu-Program, project PN 19 35 01 01 and CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCCF-2016-0006, within PNCDI III.

Section T4:

Nanostructured Materials - Nanocomposites and Hybrid Materials

Oral T4-1

Low-field NMR relaxometry investigations of cement hydration under the influence of accelerators

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Abstract. 3D printing technology may play a significant role in reducing the carbon footprint of the cement-based materials. Building without formworks has the advantage of saving the cost, time, and materials associated with formwork construction. It also allows designing of more complex structures. However, to substitute all the requirements typically fulfilled by the formwork it is necessary to develop new cement-based composites characterised by fast setting and low slump. The speed of strength development of cement mixtures can be controlled by the addition of accelerators. That is why, understanding their influence on hydration dynamics and pore evolution is important for the final characteristics of the cement-based materials. In our work, nuclear magnetic resonance relaxometry techniques are used to monitor the effect of different amounts of accelerator on hydration stages, pore size evolution and internal surface evolution. The NMR investigations are also compared with strength test, X-ray diffraction and slump tests to have a complete understanding of the accelerators on hydration process and strength development. **Acknowledgement:** This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P4-ID-PCE-2020-0533, within PNCDI III".

Oral T4-2

High performance functionalized magnetic nanoparticles with tailored size and shape for localized hyperthermia applications

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Abstract. Iron oxide (Fe_3O_4) and ferrite ($MeFe_2O_4$, Me - Mn, Zn) hydrophobic magnetic nanoparticles with various shapes and sizes were synthesized by high temperature reaction of organic precursor solution. Spherical, cubic, hexagonal and octahedral shapes and sizes ranging from 10 to 100 nm were resulted. Structurally well-formed hydrophobic magnetic nanoparticles with high saturation magnetization values were reported. Tailoring the shapes and sizes of nanoparticles allows controlling a variety of properties that are relevant to many potential applications of magnetic nanoparticles. The hydrophobic oleic acid (OA) shell was successfully transformed by a simple and environmentally friendly oxidative scission method into Azelaic Acid (AZA). The morpho-structural characteristics, size distributions, chemical composition and magnetic properties of the resulted hydrophilic nanoparticles were investigated. Magnetic hyperthermia measurements have been performed in a specially designed sample holder placed in an inductor with Cu coils assuring alternating magnetic fields of safely biological amplitude-frequency products. The optimal shape with specific size range for nanoparticles dispersed in various carriers providing the best heating efficiency is reported.

Oral T4-3

Electrocaloric effect in $BaZr_xTi_{1-x}O_3$ ceramics

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Abstract. New solid state refrigeration techniques are based mainly on two principles: adiabatic demagnetization cooling or adiabatic depolarization cooling. The last one is called electrocaloric refrigeration and it employs the electrocaloric effect (EC) of ferroelectric materials. $BaTiO_3$ (BT) family as EC materials has been studied quite extensively in the past several years and a large ΔT has been reported for BT-ceramics in the vicinity of ferroelectric-paraelectric (FE-PE) phase transition. Owing to the high transition temperature the using of pure BT as EC materials is limited, but this can be properly modified by incorporation of suitable dopants. In the present paper, we investigated $BaZr_xTi_{1-x}O_3$ ceramics with x=0.02 – 0.20. X-ray diffraction data showed the phase purity and SEM images demonstrated homogeneous microstructures. Impedance spectroscopy shows a composition-induced ferroelectric-to-relaxor crossover. All samples are tunable, DC tunability increasing with x from 2.11 (x=0.08) towards 2.6 (x=0.20) at 25 kV/cm. P(E) loops indicate regular variation with increasing Zr addition, a reducing of loop area, remanent and saturation polarization from P_{sat}=15μC/cm^2 to P_{sat}=9μC/cm^2. EC effect was indirect evaluated and a maximum of 0.7 K was obtained for x=0.04 at 373K. **ACKNOWLEDGMENTS:** The financial support of the PN III-P1-1.1-TE-2016-1951 and PN III-P1-1.1-TE-2019-1689 are acknowledged.

Oral T4-4

Supramolecular Organic Frameworks Constructed via Halogen Bonding

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Abstract. Halogen bonds are versatile tools to access diverse supramolecular architectures as host−guest complexes, macrocycles, cryptands and cages or amazing 1D, 2D, or 3D polymeric structures. They emerged as significant driving forces for supramolecular self-assembly, gaining great interest during the last two decades. In this context, supramolecular assemblies of 2,7-dipyridylfluorene and Halogen-Bonded Organic Frameworks (XBOF) respectively, formed by N---I contacts of pyridyl N atoms with pentafluoroiodobenzene or diiodotetrafluorobenzene isomers were obtained by mechanochemical synthesis. Their structures were determined by single crystal X-ray diffraction. The contribution of specific noncovalent interactions between different building blocks to the stability and solid-state packing behaviour of the supramolecular polymers was evaluated by theoretical calculations, which confirm the geometries and interactional bonding observed in single crystal X-ray diffraction structures.

Oral T4-5

MOF(Al) based catalysts for CO_2 methanation

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Abstract. The exceptional structural properties of metal-organic frameworks (MOFs), such as their very large surface area, their tunable porous structure, or their capacity to adsorb and store gaseous molecules, to name but a few, have opened the gate for their enhanced use in heterogeneous catalysis. Among the numerous catalytic applications thereof, use of MOFs in the methanation of CO_2 is motivated by the possibility to enhance the activation of both reactants used in the process: (a) activation of CO_2 is favoured by the special porous structure, while (b) activation of H_2 might be achieved due to the increased metal dispersion on the support, as a consequence of the exceptional surface area. In this work, we report on the use of aluminum-based MOFs as catalytic supports in the methanation of CO_2 at low reaction temperatures (<400°C), with Ni nanoparticles embedded in the porous structure of the MOFs.

Oral T4-6

Bioinspired hybrid materials for cancer therapy

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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 bioinspired polydopamine has entered the field of nanomedicine as a versatile coating for nanomaterials vesting them photothermal properties. In this talk, we present synthesis of multifunctional nanocariiers based on polydopamine coated magnetic nanoparticles with PAMAM dendrimers equipped with targeting moiety as well as PDA particles for combined chemo- and photothermal therapy of liver cancer. The research was financed by the National Centre for Research and Development under research program LIDER/11/0055/L-7/15/NCBiR/2016.

Oral T4-7

Voltage control of perpendicular magnetic anisotropy in systems displaying quantum well effects

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Abstract. Magnetic thin films with perpendicular magnetic anisotropy (PMA) represent an important building block in non-volatile information storage. The proper control of this parameter is crucial for memory device reliability and energy efficiency. The PMA needs to be large enough to withstand thermal fluctuations, but moderate enough in order to allow the magnetization manipulation with a reduced energy consumption. A low energy magnetization reversal of a few fJ/bit and sub-ns switching times can be achieved by controlling the magnetization using an electric field. In this context, our work represents a theoretical *ab-initio* study of the PMA and its variation with the applied electric field in *X*/Fe/MgO(001) multilayer configurations (*X* = Cr, Au, V) compatible with standard experimental architectures of magnetic tunnel junction devices. Our aim is to describe, quantify and underline the significant role of the Rashba interfacial field at both bottom *X*/Fe and top Fe/MgO interfaces on PMA, as well as the implications of the anisotropy oscillations, observed when varying the number of Fe layers, previously explained within the framework of quantum wells of the Δ_1 Bloch symmetry Fe electrons.

Oral T4-8

Modeling the complex dielectric properties in ferroelectric-based composites by a dynamic finite element method

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Abstract. Since single-phase ferroelectric materials cannot accomplish all the technological requirements in applications, developing composite materials that combine the properties of the ferroelectrics with other constituent phases (linear dielectrics, magnetic materials or other conductive/ semiconductor components) is a commonly proposed solution. Recently, it has been shown that a major factor that influences the effective properties of composite materials is the local electric field inhomogeneity introduced by the interfaces. Based on this effect, we proposed the original concept local field engineering which involves the design of materials with controlled microstructures and, implicitly, an optimum inhomogeneity of the electric field to improve the functional properties. Another important factor that influences the functional properties of composites is the accumulation of free charges at interfaces, but this has been neglected so far because it involves important computational difficulties. In this work we propose a new modelling dynamic approach based on finite element method able to describe the complex impedance at any frequency in the range from 1Hz to 1MHz. The approach allows us to explore the influence of free electric charges on the effective dielectric properties of real composite systems as ferroelectric-semiconductor, magnetoelectric, porous ferroelectrics, etc. Acknowledgment: UEFISCDI project PN-III-P1-1.1-TE-2019-1929.

Oral T4-9

Decoherence in fluxonium based superconducting circuits

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Abstract. Quantum circuits based on superconductors gained huge popularity due to the flexibility in tailoring their Hamiltonian. We evaluated and characterised an artificial atom based on fluxonium qubit architecture, focusing on the regime in which the external flux is half of flux quantum, which minimizes the flux noise. We studied the interaction of our system to the environment when coupled to a readout resonator. We were able to calculate the relaxation rates for various relaxation mechanisms, and compared them to those for a typical fluxonium qubit.

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Oral T4-10

Linear response theory for non-Hermitian systems

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Abstract. Linear response theory has a large applicability in physical sciences as it often gives the leading order response of a system to an external probe. We develop an extension of the theory to the domain of non-Hermitian quantum mechanics, where wave functions have a non-unitary dynamics. We exemplify the salient features of this theory through two examples which contain surprising predictions for the behavior of expectation values in the non-Hermitian realm: 1) finite electrical dc conductivity in a one-dimensional tachyon system and 2) absence of Friedel oscillations due to an imaginary potential.

Poster T4-1

Investigation of TiO_2/3D free-standing graphene networks

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Abstract. Over the time, the semiconductors were considered as very interesting materials for application in sensing devices, solar cells, energy storage and conversion. One of these materials is TiO_2, an environmental-friendly material having high chemical and thermal stability and photostability, which is particularly suitable for photocatalysis, energy storage and a wide range of other applications. In recent years, graphene-TiO_2 nanocomposites have attracted much attention due to their extraordinary characteristics, i.e., the photocatalyst activity enhancement and the accelerated electron mobility to reduce the charge recombination. Graphene-TiO_2 composites show high interfacial contact and potential to enhance the photocatalytic activities of TiO_2. In this research, we develop TiO_2/3D free-standing graphene networks. The 3D graphene networks were obtained by chemical vapour deposition technique on commercial nickel foam with methane as carbon source at 1000°C under ambient pressure and the TiO_2 thin films were deposited by electron beam evaporation from TiO_2 granules. The obtained TiO_2/3D free-standing graphene networks were investigated by SEM, XRD, EDX and UV-Vis. **Acknowledgments:** This work has received funding from the Bilateral Collaboration Romania-Russia, project position 28 from the JINR Order no. 365/11.05.2021.

Poster T4-2

Comparative study of the hydrophobic properties of silica nanoparticles functionalized with different agents

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Abstract. In this paper is presented a comparative study of the hydrophobic properties of silica nanoparticles functionalized with different agents. The main properties of highly hydrophobic surfaces are weak water adhesion and self-cleaning behaviour. Different silane precursors were used in order to develop superhydrophobic surfaces by sol-gel method. Spherical silica nanoparticles were synthesized by a sol-gel process and the modification of their surface was performed by a functionalization process with different silanes (hexamethyldisilazane-HMDS and perfluorooctyltrichlorosilane-PFOTS). The hydrophobic properties were evaluated by measuring the water contact angle. The resulting values of the water contact angle for all the analysed samples are higher than 140°, this fact confirming the hydrophobic character of the functionalized silica nanoparticles. **Acknowledgments:** This work was supported by the Competitiveness Operational Programme, subsidiary ctr. no. 133 D4 ROSEAL/2018.

Poster T4-3

Spectroscopic and microscopic investigations of the graphene oxide influence on hybrid powder products based on LDH structures

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Abstract. This work investigates a complete morpho-structural characterization of new composites based on $Mg_3Al_{0.75}Ce_{0.25}$ (Ce-doped LDH) and graphene oxide (GO) in various concentrations using Raman spectroscopy, an important tool able to assess defects in hybrid powders and display the presence of GO in their composition. Scanning electron microscopy (SEM) was employed for the structural characterization of the new compounds and the identification of the GO crystallization process and their interaction with Cerium modified LDH composites. Energy-dispersive X-ray (EDX) spectra also validated the Raman results. The similar morpho-structural defects regardless of GO concentration in the doped hybrid powders indicates that the amount of GO used in our samples can be successfully integrated into novel composites with enhanced mechanical properties. **Acknowledgments:** This work was supported by a grant of the Romanian, Ministry of Research, Innovation and Digitization CCCDI – UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0387 / 80PCCDI⁄2018, within PNCDI III.

Poster T4-4

Anticoagulant properties of coated Fe-Pd ferromagnetic shape memory ribbons

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Abstract. Ferromagnetic shape memory alloys are interesting new materials for the manufacture of stents. Their shape-changing ability allows them to be used as a self-expanding device based on temperature or magnetic field, without the need of additionally introduced mechanical force like in balloon angioplasty. Iron-palladium alloys in particular can be used to manufacture temporary stents due to their optimum rate of degradation. In order to avoid blood clotting upon introduction of the stent, they are often coated with anticoagulants. In this study, sulfated pectin, a heparin mimetic, was synthesized in different ways and used as coating on multiple iron-palladium alloys. Static and dynamic PT and APTT of the prepared materials were compared to samples uncoated or coated with polyethylene glycol. APTT increased significantly with all alloys coated with sulfated pectin. Aside from that, sulfated pectin synthesized by different methods also caused slight changes in APTT. These findings show that iron-palladium alloys can be coated with anticoagulants to improve their utility as material for temporary stents. Sulfated pectin was characterized by NMR and FTIR, and the coated alloys by SEM and EDX.

Poster T4-5

Transparent thin film of zinc oxide for solar cells applications fabricated by pulsed laser deposition

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Abstract. The most common material used in the construction of photovoltaic cells is silicon. In order to reduce the production costs, new methods are developed to create thin layer cells, whose composition includes cheaper materials from the point of view of the manufacturing process in comparison with pure silicon. Zinc oxide (ZnO) thin film used as n-type transparent conductive oxide (TCO) layer in heterojunction devices is a promising semiconductor material for advanced optoelectronic applications due to its wide direct band gap (3.37 eV), large exciton binding energy (60 meV), high electron mobility, good transparency, high thermal and mechanical stability, low cost, non-toxicity and demand to relatively low deposition temperature. Solar cells production using n-type ZnO thin films grown on p-type Silicon (Si) are of great interest nowadays. By employing pulsed laser ablation technique (PLD) we envision a cheap and sustainable method in order to obtain a high efficiency heterojunction n-ZnO/p-Si. N-type conduction of ZnO is usually due to presence of defects in ZnO lattice, mainly zinc interstitial atoms that act as active impurity donors.

Poster T4-6

Structural and electrical properties of $Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$ ceramics

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Abstract. In the past decade the lead-free ceramics, especially $(Ba,Ca)(Ti,Zr)O_3$ ceramics, have attracted a broad interest as lead-free piezo/ferroelectric ceramics. In the present paper, we compare the properties of two types of $Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$ (BCTZ) ceramics, the morphotropic phase boundary composition, sintered from 2 types of powders produced by mixed oxides method by using the same precursors, but following different calcination procedures, follow by the same temperature of 1450°C/4h. The X-ray analyse has revealed the formation of pure perovskite phase and the coexistence of superposition of phases (orthorhombic and tetragonal). It was performed a comparative study at the low and high electric field (dielectric constant vs. temperature and frequency, P(E) hysteresis loops and dc-tunability) for both investigated BCTZ ceramics. The effect of electric poling on the structural and piezoelectric properties of the BCTZ samples was analysed and discussed. **Acknowledgements**: This work was supported by Romanian Ministry of Research and Innovation grant, CCCDI-UEFISCDI, project no PNIII-P3-3.1-PM-RO-FR-2019-0069.

Poster T4-7

Effect of sintering on structural and electrical properties of (Ba,Sr)(Zr,Ti)O_3 ceramics for energy storage applications

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Abstract. The $SrTiO_3$ (ST) and $BaZr_{0.15}Ti_{0.85}O_3$ (BZT) powders were combined and prepared through the solid state reaction method. The mixt 5%ST+95%BZT compound was sintered at different temperatures, from 1350°C to 1500°C, and the effect of sintering temperature on structural and electrical properties has been studies. The X-ray diffraction investigation of the ST, BZT and the composites ceramics, confirmed the formation of pure perovskite phase with a cubic structure. The functional properties (dielectric, ferroelectric and non-linear properties) were investigated and discussed. The efficiency and energy storage were calculated from P(E) hysteresis loops and they have shown that the ST-BZT composites present higher storage energy and efficiency than in ST and BZT ceramic, which are making them suitable for energy storage applications. **Acknowledgment**: This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS – UEFISCDI, project no PN-III-P4-ID-PCE-2020-1988, within PNCDI III

Poster T4-8

From macro to nanoLDPE: crumbling/grinding time and impact on bacteria

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Abstract. LDPE (Low Density PolyEthylene) bags that are massively produced and discarded throughout the world end up in terrestrial and aquatic ecosystems. It was proven that plastic is reduced to micro dimensions and many speculate that LDPE could be degraded to nano-dimensions, but no certain data was provided in this regard. This work was aimed to show how only 10 days of exposure to UVC light are enough to produce nanoLDPE which interacts with chemo- and photosynthetic bacteria. Through scanning and transmission electron microscopy, Raman spectroscopy, FTIR, and confocal microscopy the interaction between nanoLDPE and microorganisms was observed. A short-term exposure of 72 h was sufficient to affect the growth rate of *Arthrospira platensis* and to inhibit the development of *Escherichia coli* bacteria. Considering that LDPE environment pollution began less than 50 years ago, a series of concerns are raised regarding how we can downsize the damages that may have occurred.

Poster T4-9

The influence of pH on the stability of SiO_2 suspensions

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Abstract. Nanomaterials are currently widely used due to the various processing possibilities for a wide range of applications. SiO_2 nanoparticles (*NPs*) attracted extraordinary attention in scientific research domain due to the posibility of design with specific tailored properties for targeted medical applications. Stöber method has been used since 1968 and with same minor modifications, is the most widely used method for synthesis nanometric SiO_2. Due to their geometry and size, the SiO_2 *NPs* are suitable for 3D printing technique (used in the case of medical applications, in bone tissue engineering), a very modern method for materials processing. For this purpose, the SiO_2 *NPs* are used in suspensions and it is very important to know the *NPs* surface loading, due to its major influence on their aggregation behavior. The currently used methods do not allow the accurate measurement of this property, this being estimated from corresponding the zeta potential. In this study we present the pH influence on the stability of the SiO_2 suspensions. The SiO_2 NPs were prepared by the classic Stöber method, with spherical uniform geometry and size of 120 nm. To determinate the zeta potential were prepared suspensions with 0.05 wt % SiO_2 in various pH solutions: 1.679, 4.00, 7.00, 10.00 and 12.45. In the case of basic pH the values of the zeta potentials were bigger then -30mV, indicating that analyzed suspensions present stability in this medium. **Acknowledgments:** This work was supported by the Competitiveness Operational Programme, subsidiary ctr. no. 133 D4 ROSEAL/2018.

Poster T4-10

One step hydrothermal synthesis of nitrogen, boron co-doped graphene

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Abstract. In this work, we synthesized nitrogen and boron co-doped graphene by one step co-doping using the hydrothermal method with graphene oxide (GO), urea and boric acid as the carbon precursor and heteroatom sources. The effect of the reaction time, temperature and the GO: urea: boric acid ratio was thoroughly investigated by SEM, X-Ray powder diffraction, FTIR and XPS. The influence of nitrogen and boron co-doping on the morphology, structure, and composition of the NB-Gr was systematically investigated, and the results show that urea and boric acid coexisting in the hydrothermal system not only act as the N and B doping sources but also as catalysts to boost the synergistical doping of N and B. **Acknowledgment**: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, project number PN-III-P4-ID-PCCF-2016-0006, within PNCDI III.

Poster T4-11

Preparation and characterization of hybrid materials based on graphene oxide and enzymes

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Abstract. Enzymes are proteins that act as biocatalysts, having an important role on an industrial scale. The major disadvantage of enzymes is their facile denaturation. By obtaining hybrid materials based on immobilized enzymes on graphene oxide and reduced graphene oxide we target an increase in the stability and activity of enzymes. In this study we successfully prepared hybrid graphene oxide and reduced graphene oxide materials with immobilized porcine pancreatic lipase and candida rugosa lipase. We used the *non*-covalent immobilization method which involves the physical absorption of the enzyme on the substrate. The successful immobilization of three different lipase enzymes on graphene oxide was demonstrated by detail characterizations using X-ray diffraction, FTIR, solid UV-VIS spectroscopy, liquid UV-VIS spectroscopy, TEM, SEM, TGA in air and argon.

Poster T4-12

Wearable and disposable sensors for wound infection biomarker monitoring

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Abstract. Wound infections pose a significant threat to the wound healing process, being one of the most serious complications that can occur in wounds, irrespective of wound etiology. Current methods of infection diagnosis rely mostly on clinical inspection or microbiological analysis. Both of these approaches present serious limitations, such as a high degree of inaccuracy for clinical inspection, and long analysis times in the case of laboratory cultures. A promising alternative for early diagnosis of wound infection is represented by the detection of certain biomarkers, such as bacteria metabolites, enzymes, inflammatory mediators, physio-chemical parameters (pH, oxygenation, temperature changes) or even the detection of bacteria itself. An ideal way to reduce patient discomfort during the diagnostic procedure would be to integrate sensors for biomarker detection directly into the dressing used for wound protection and treatment. To this aim, wearable and disposable sensors have been developed in recent years. In this contribution we will be discussing the latest achievements in the field of wearable and disposable sensors for wound infection biomarker monitoring. **Aknowledgement:** A. Pusta acknowledges UMF internal grant no. 1032/57/13.01.2021.

Poster T4-13

Eco-friendly method for PGM recovery from spent auto converters

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Abstract. Every car with an internal combustion system has to be equipped with a catalytic converter in order to reduce the impact of the exhaust gases on the environment. The gasses are converted by employing a catalyst based on platinum-group metals (PGMs), especially platinum (Pt), palladium (Pd), and rhodium (Rh). The demand for these materials is increasing and the natural resources are diminishing. Therefore, a solution could be the recycling of the catalytic converters for the recovery of PGMs as pure metals. However, the recovery of the PGM is not an easy process since the composition of catalytic converters is very complex. In this study, we established an eco-friendly laboratory method for recovering of the PGM by varying different experimental conditions such as: HCl/H_2O_2 (as a leaching solution) ratio, temperature, and contact time. Furthermore, different precipitation techniques were employed in order to separate the individual ions from the leaching solution and to obtain high yield and purity for recovered Pt, Pd.

Poster T4-14

On the Resonance Raman excitation of Zinc Oxide nanoparticles

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Abstract. Zinc oxide (ZnO) nanoparticles (NPs) coated or decorated with Au of Ag nanostructures are a perspective substrate for Surface-enhanced Raman scattering and Surface-enhanced fluorescence applications. Raman spectroscopy (RS) is one of the methods of choice for structural analysis of the ZnO NPs; however, the proper evaluation of sample properties is not yet established, due to certain knowledge gaps and non-equivocal literature claims on the behaviour of spectral features under resonant and non-resonant excitation. We synthesized a series of ZnO NPs of different morphologies (spherical, polyhedral, flowers), with plasmonic resonances between 330-370 nm. The NPs were analysed by RS under non-resonant 532 nm and pre-resonant 442 nm excitation, respectively. The bands showed mode-specific broadening, shifts, and enhancement. Furthermore, a green photoluminescence band around 460 – 463 nm was observed. The relationships and origins of the spectral changes when passing from the non-resonant to pre-resonant excitation are discussed here and we provide a contribution towards efficient and precise structural analysis of ZnO NPs via advanced spectral interpretation.
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Poster T4-15

Hyaluronic acid @ Polydopamine composite coatings: synthesis and characterization

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Abstract. Polydopamine (PDA) is regarded nowadays as an almost universal surface modification agent due to its strong adhesion to virtually any substrate, on the one hand side, whereas on the other hand side, to its capacity to bind many types of functional molecules, including large biomolecules. Here, we report the results of a systematic study aimed at determining the specific conditions for incorporating hyaluronic acid (HA) into the PDA matrix, in particular the oxidation conditions and the dopamine *vs* HA relative concentrations. The possibility of forming robust HA@PDA composite coatings will be probed at molecular scale by solid-state NMR spectroscopy, whereas the thickness and surface topography of the depositing layer will be investigated by Atomic Force Microscopy (AFM). The obtained data will be correlated with the purpose of introducing a reliable methodology for the quality control of the deposited HA@PDA thin film, which is a necessary initial step in the perspective of the potential biomedical applications of this composite material, for instance in implantology.

Poster T4-16

Neoteric Clay-Based Material for Heavy Metals Removal from Mining Waters

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Abstract. The acceleration of urban development and the continuous population growth has dramatically increased the contamination of waterbodies with heavy metals, toxic anions or organic pollutants. As a result, scientists focused on developing new "environmentally-friendly" materials for adsorption procedures to eliminate various pollutants from wastewaters. Herein, we report the preparation of a neoteric clay-based material, obtained from montmorillonite and functionalized poly(benzofurane-*co*-arylacetic) acid, able to complex metal ions. Various analytical techniques such as SEM, TGA, XPS, FTIR and AAS were applied to investigate the structure, morphology and chemical composition of the synthesized material and the heavy metals content. Stock solutions of Cu^{2+}, Zn^{2+}, Mn^{2+}, Fe^{3+}, Pb^{2+}, Cd^{2+}, Cr^{3+}, Ni^{2+} and contaminated water samples collected from Roșia Montană Mining Area were used to evaluate the material's suitability for metals removal from wastewaters. **Acknowledgements.** This work was supported by Ministry of Research, Innovation and Digitalization through Core project PN-19-35-02-03, No. 36N/13.02.2019.

Poster T4-17

Selective Hydrogen production from formic acid decomposition on reduced graphene oxide supported AuPd nanocomposites

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Abstract. Hydrogen (H_2) is considered a feasible and environmentally attractive energy carrier, although efficient and safe hydrogen storage technologies under mild conditions need to be developed. A feasible option is the storage of H_2 in an organic liquid medium (*Liquid Organic Carriers*, LOC) which can release H_2 in situ at ambient temperature for direct use in fuel cells. For the recent years, Formic Acid (FA, HCOOH) a major product of biomass processing, has been investigated as promising liquid storage material, capable to release hydrogen under mild condition via a catalytic decomposition. FA, is nontoxic and a liquid at room temperature, with a density of 1.22 $g \cdot cm^{-3}$ which contains 4.4 wt. % (53g/l) of H_2. An important strategy to promote the development of hydrogen generation from formic acid is the use of new heterogeneous catalysts with high activity and relatively low cost, designed to replace the homogeneous catalysts with difficult synthesis, separating and recycling. In this study we present the facile synthesis of mono-metallic Pd(10wt%), Au(2.5wt%, 5 wt% and 10wt%) and bi-metallic Pd(7.5wt%)-Au(2.5wt%) alloy nanoparticles supported on reduced graphene oxide (rGO) by a new, simple, accessible and environmentally friendly method and investigation of their catalytic properties for FA decomposition in aqueous solution.

Poster T4-18

New emerging magnetic properties of FePt@SiO_2 nanocomposites

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Abstract. Magnetic nanocomposites based on FePt (half-metal) as core and SiO_2 as shell having new emerging properties were obtained, by chemical route, in two steps: (i) first FePt phase was prepared from precursor of iron (iron pentacarbonyl-Fe(CO)5) and platinum (platinum II acetylacetonate - Pt(C5H7O2)2), (ii) then the cores were covered with SiO_2 shells by a son-chemical method using tetraetoxysilane as silicon precursor. The sample composition was determined by XPS, the structure was checked by XRD and TEM analyses while the energy bans alignment was evidenced by UPS. The magnetic properties were investigated by VSM magnetometry. When a half-metal ferromagnetic material is interfaced with a semiconductor there is a polarized charge / spin transfer between the ferromagnet (FePt) and the semiconductor (SiO_2). As a result, ferromagnetic ordering of single occupied defects and vacancies in SiO2 will result at all temperatures. The nanocomposite will show higher saturation magnetization and higher coercivity than the FePt stand-alone nanoparticles. A discussion about the above mechanism is done.
Acknowledgements. This work was supported by the Romanian Ministry of Research, Innovation and Digitization, Core Programme, Project PN19 35 02 03.

Poster T4-19

Study of the Interphase Exchange Coupling and Magnetocaloric Effect in Co_3Gd_4+Co_7Gd_{12} Nanocomposite Obtained by Mechanical Milling

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Abstract. The magnetic phases Co_3Gd_4 and Co_7Gd_{12} were obtained by arc melting. The as-cast ingots were annealed to ensure homogeneity. X-Ray diffraction studies have shown that the ingots are single phase with the hexagonal structure ($P6_3/m$) and monoclinic structure (P21/c), respectively. Thermomagnetic measurements have shown their Curie temperatures to be 220 K and 163 K, respectively. The magnetic Co_3Gd_4/Co_7Gd_{12} nanocomposite powders were produced by the mechanically milling (MM) of crushed and sieved powders obtained from the alloys. The MM process was followed by annealing to improve the microstructure of the nanocomposite. The relationship between the interphase exchange coupling and the microstructure was investigated by magnetic measurements and X-Ray diffraction. The magnetic entropy change was studied in the nanocomposite materials and the component phases. The magnetic refrigeration efficiency was evaluated by calculating the relative cooling power (RCP) for the investigated nanocomposite. **Acknowledgement**: Financial support of Babeș-Bolyai University, grant GTC35273/18.11.2020

Poster T4-20

New magnetic polymeric hybrid composite electrode material for amperometric nitrite sensor

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Abstract. New modified electrode materials, based on a combination of hybrid nanocomposites such as magnetic nanoparticles, inorganic polymer, like silica and organic polymer like poly acrylic acid (pAac) ((MNPs-SiO2 and MNPs-SiO2-pAAc) were studied. The as prepared magnetic polymeric composite materials present high potential applicability as electrochemical sensors for quantitative measurements of nitrite from different kind of real samples.

The electrochemical properties of the synthesized materials were investigated. By electrochemical measurements was proved that this electrode presents electro catalytic effect towards nitrite oxidation and can be used for nitrite detection. By comparing with other electrodes, the electro catalytic effect of MNPs-SiO2-pAAc is better, because the nitrite oxidation peak appears in this case at a potential closer to 0 mV vs. Ag/AgCl/KClsat, which is favourable to avoid interferences in amperometric nitrite detection in real samples

Poster T4-21

The influence of alcohol in mouthwash on a bone regeneration cement: NMR relaxometry investigations

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Abstract. The presence of alcohol in mouthwash may kill superficial bacteria in the oral cavity but may also damage the fillings and dental restorations. The studies show that non-alcoholic mouthwash is more beneficial for the luster, colour, hardness, and wear of restorations. The present work analyses the influence of alcohol in mouthwash, applied in daily use, for two experimental cements designated for bone regeneration. The cements contain two phases: organic (UDMA, PEG, HEMA) and inorganic (TCP with and without chitosan) with chemical initiation system (POB / DHEPT). The samples, hardened by the polymerization reaction, are stored in two different media: alcoholic mouthwash and non-alcoholic mouthwash, from the same producer. To investigate the absorption, the studies involved storing and weighing the samples at different time intervals. Furthermore, the pore evolution, and the absorption dynamics were also monitored by low field nuclear magnetic resonance relaxometry. The results show that absorption influences both the degradation of the cement over time and the pore connectivity of the regeneration cement.

Poster T4-22

New Drug Carrier for Slow Release: 5-Fluorouracil Formulation in Nanoporous Biogenic Mg-calcite from Blue Crab Shell

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Abstract. The extraordinary evolution of nanotechnology, has established the field of nanomedicine as a focal point of scientific innovation. In the present study, the porous 3D nanostructure of the biogenic calcium carbonate, from wasted blue crab shells, has prompted its use as a drug carrier for 5-fluorouracil, a drug widely used in cancer therapy. A drug solution was prepared and loaded subsequently in the pores of the biogenic powder, and further pressed into tablets. The surface structure and composition of the tablets has been investigated using a series of different techniques: Confocal Raman Spectroscopy, X-Ray Diffraction (XRD), Scanning Electron Microscopy, with the results clearly showing that the drug is adsorbed in the pores of the biogenic carrier. The slow release of the drug from the tablet was investigated by tracking and quantifying the Surface Enhanced Raman Scattering signal of the tablet solution in a series of time dependence experiments. The proof of concept is thus demonstrated by quantifying the slow release of the drug in a time course of 26 hours. The results showed great promise for re-using waste biogenic materials of aquatic origin as drug carriers, in line with the concept of blue bioeconomy.

Poster T4-23

Synthesis, characterization and photocatalytic activity of MWCNTs decorated with Cu-doped TiO_2

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Abstract. The decoration of MWCNTs with TiO_2 and transition metal doping can induce - charge transfer and enhance the photocatalytic activity of TiO_2. MWNTs decorated with TiO_2:Cu nanoparticles were prepared by a polymer wrapping-technique. At a constant MWCNTs : TiO_2 ratio, the Cu doping (x=0,1,3,5,7%) 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 percentages of RhB degradation varies between 45-89%, whereas the best photocatalytic activity obtained for 1% Cu doping. The results revealed that by Cu doping one can control the decoration efficiency and photocatalytic activity.

Poster T4-24

CNT-COOH/MnO_2/Fe_3O_4 nanocomposite as adsorbent for the removal of pesticides from aqueous solution

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Abstract. The pesticides are substances widely used in agriculture to protect plants from weeds, insects, and other pests, but despite of the benefits, pesticides can persist long term in the environmental compartments and causes significant problems for ecosystems. . For these reasons, their removal from water sources is urgent. Carbon nanotubes (CNTs) and metal oxides are the new generation of materials with improved properties. These not only combine the properties of carbon nanostructures and metal oxides, but also have new properties due to their interaction. These nanocomposites have large and chemically inert surfaces with a relatively uniform structure, providing multiple sites of adsorption. In this study, the application of CNT-COOH/MnO_2/Fe_3O_4 nanocomposite to remove the devrinol, used as pre-emergence herbicide, and triadimefon, a good protectant and eradicant fungicide against powdery mildew and rust fungi, was investigated. In this regard, a series of physico-chemical parameters (pH of solutions, temperature, adsorbent dose, contact time and initial concentration of pesticide) was tested to obtain the highest possible removal degree of the selected pesticides from aqueous solution. **Acknowledgments:** This work was carried out through the Romanian Ministry of Research, Innovation and Digitization within the Core Program, PN19-35-0203 (36N/13.02.2019).

Poster T4-25

Pulsed laser deposition of ZnS/FePt thin films on Mg (100) substrates

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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 magnetic properties were measured by VSM magnetometery with in-plane and out of plane configuration. The deposition parameters were for FePt: P=4.3 x 10^{-2} mbar, Ar atmosphere, T=700^{o}C, 9600 pulses, 5 Hz. For ZnS the deposition parameters were: P=5.8 x 10^{-2} mbar, Ar atmosphere, T=450^{o}C, 1200-2400-4800 pulses, 5 Hz.

Poster T4-26

Green preparation and applicability of chitosan/carbon based nanomaterial in Sunset Yellow electrochemical detection

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Abstract. Food additives are normally used in processed foodstuff to enhance appearance, flavor, taste, color, texture, nutritive value and preservation. Synthetic colorants containing azo functional groups (N=N) and aromatic ring structures have been widely used to replace natural food color in food industry. However, it is necessary to note that such synthetic colorants are able to affect human health being pathogenic, particularly when they are excessively consumed. Therefore, their detection in a rapid, sensitive and simple manner is quite important for human health and food safety. The main goal of this study was to provide a facile, rapid, inexpensive way for the green, one-step and large-scale preparation of chitosan/carbon based nanomaterial, through electrochemical exfoliation of graphite rods, without the use of any organic solvent. Moreover the applicability of chitosan/carbon based-glassy carbon modified electrodes for accurate detection and quantification of Sunset Yellow from commercially available food and beverage products was tested.**Acknowledgement** This work was supported by grants of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number number PN-III-P2-2.1-PED-2019-2410 (500PED/2021) and PN-III-P4-ID-PCCF-2016-0006 within PNCDI III.

Poster T4-27

The influence of the vacuum plasma treatment on the cotton surface deposited by Tio_2 / Tio_2+graphene nanopowder water colloidal dispersions

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Abstract. This work presents the influence of the vacuum plasma treatment on the deposited surfaces of cotton samples by their immersion in TiO_2 and TiO_2+graphene water colloidal dispersions. The immersion process in bi-distilled water dispersions of TiO_2 and grapheme-based nanomaterials took place in ultrasound bath. Before and after immersion the deposited samples were preceded or followed by vacuum plasma treatment using air as working gas. The SEM-EDS analyses show different degrees of immobilization for TiO_2 and TiO_2+graphene on the cotton substrates, dependent on the treatment method. For both TiO_2 and TiO_2+grapheme immersion it can be observed that the highest amount of Ti can be found in the non-treated samples. The lowest amount of Ti was found, in both sets, in the samples that underwent plasma treatment before and after immersion probably due to removal of less adhesion nanoparticles and remaining of the more adherent ones. The preliminary RBS evaluations show higher amount of Ti for the samples treated both before and after immersion. These investigations lead to an interpretation of a higher degree of immobilization of the nanopowders, even in lower amounts, on these treated surfaces.

Poster T4-28

Quantum transport through a quantum dot coupled to a Majorana ring

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Abstract. We theoretically investigate quantum transport through a quantum dot coupled to Majorana bound states connected at the ends of a topological superconductor nanowire threaded by a tunable magnetic flux. We show that when the two Majorana bound states do not overlap, the linear conductance has a 2π periodicity as a function of magnetic flux phase, independent of the quantum dot energy, or the finite values of dot-Majorana couplings. In the case when the Majorana bound states overlap, the linear conductance periodicity transforms to 4π due to dot level energy which is tuned away from the Fermi level. Therefore, differential conductance periodicity changes from 2π to 4π when the Majorana bound states are not perfectly degenerate. Our results provide insight into Majorana-induced transport signatures. **Acknowledgments.** L. M. and D. S. were supported by a grant of the Ministry of Research, Innovation and Digitalization, CNCS/CCCDI – UEFISCDI, under project number PN-III-P1-1.1-TE-2019- 0423, within PNCDI III.

Poster T4-29

Nanotoxicity of graphene materials on A375 and HaCaT cell lines

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Abstract. The wide scale use of nanoparticles (NPs), due to their unique properties, makes human being more prone to its potential adverse effects. Therefore, the aim of the present study was to investigate the effects of graphene oxide nanoparticles complexed with titanium dioxide and copper or copper oxide (TiO_2/CuO/GO and TiO_2/Cu/TRGO) on A375 and HaCaT cell lines exposed to visible light. We explored the cytotoxicity and oxidative stress induced by nanoparticles. Cell viability, nitric oxide levels and extracellular release of lactate dehydrogenase were assayed in cells after 24 hours incubation with 0.01-1 mg/ml treatments. The results showed that nanoparticles under light iradiation reduced cell viability, induced nitric oxide generation and impaired cell membrane integrity of cells in a dose dependent manner. It is valuable to inform that HaCaT cells appeared to be slighty more susceptible to TiO_2/CuO/GO treatment than A375 cells. These results provide a basic comparative toxic effect of TiO_2/CuO/GO and TiO_2/Cu/TRGO nanoparticles on normal keratinocytes and cancerous epitelial cells. **Acknowledgements**. This work was supported by grants of Project RO-NO-0616, contract no. 29/2020 and Project PN-III-P1-1.2-PCCDI-2017 0743/44PCCDI/2018.

Poster T4-30

Current progress and perspectives on biomaterials used in surgical applications

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Abstract. Recent advances in the development of biomaterials have given new options for surgery. There new generation of medical devices controlle chemical breakdown and resorption, prevent post-operative adhesion and stimulate regeneration of tissues. These biomaterials include a diverse array of medical devices, including non-degradable biomaterials (silicone, polypropylene, expanded polytetrafluoroethylene etc) or biodegradable polymers. including implants and three-dimensional scaffolds for tissue engineering, which require particular physicochemical and biological properties. Based on the combination of new generation technologies and cell-based therapies, the biocompatible and bioactive properties of some of these medical products can lead to progress in repair of injured or harmed tissue and in tissue regeneration. The paper provides a review of biomaterial-based treatment and prevention methods used in surgical applications and discuss the perspective in the development of innovative biomaterials.

Poster T4-31

Skin Cells Photooxidized with Titanium Systems Excited with VIS Light

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Abstract. The interest for nanoparticles (NP) increased in the last years thanks to their unique proprieties and wide use. In this study, the effects of graphene NP doped with titanium dioxide (TiO_2) and silver (Ag) or copper (Cu) were assessed on the 375 and HaCaT cell lines, in the absence and presence of visible light. Cytotoxicity and oxidative stress were investigated with the help of three assays: cell viability, the quantity of lactate dehydrogenase released and the level of nitric oxide. More precise, the cell lines were treated with two mixtures (TiO_2/Ag/TRGO and TiO_2/ Cu/TRGO) at five concentrations and incubated in the absence or presence of visible light and after that, the specific assays were made. The findings of this research proved that the toxicity induced by the NPs damaged the A375 cell line much more compared to the HaCaT cell line. In addition, the results also showed that high concentrations of TiO_2/Ag/TRGO had the most aggressive effect. This study proved the antitumoral effect of NPs doped with the mixtures, but, due to the fact that the NPs used are known to be present in everyday products, further studies are recommended to be made on the HaCaT cell line. **Aknowledgements:** This work was supported by the following grants: Project RO-NO-0616, contract no. 29/2020 and Project PN-III-P1-1.2-PCCDI-2017 043/44PCCDI/2018

Poster T4-32

Behavior analysis of two-component waterproofing mortars by mechanical and NMR investigations

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Abstract. Advanced ^{1}H NMR relaxometry becomes more and more important tool used for the characterization of a large range of materials like mortars. CPMG pulse sequence and saturation recovery methods were used for the measurement of four samples (MF, C166, P288, AQSE) of two-component waterproofing mortars at 1, 3, 7, and 28 days after preparation. In general, four dynamics components were observed for the T_2 Laplace distributions except for T_2-distribution measured for MF sample at 1 day after preparation. Their characterization reveals the dynamics and mobility of protons. In general, at low T_2 values these peaks can be associated with bound water. The flexural tensile strength and compressive strength were measured for all samples and the mechanical properties were correlated with NMR parameters. The hydrating behavior of the two-component waterproofing mortar dried under natural conditions was observed and the hydrophobic capabilities were evaluated.

Poster T4-33

Modeling the interaction between bacteria and 2-D nanoflakes

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Abstract. The interaction between 2-D nanoflakes and bacteria in water based physiological liquids is a hot topic both as it unveils new types of phenomena and since it is at fundament of many 2-D materials applications to biosciences.In this work we extend the theory named after Derjaguin, Landau, Verwey and Overbeek (DLVO theory) that describes the behaviour of nano-objects in solutions, to the case of 2-D nanoflakes interacting with bacteria cell membranes, both for gram-positive and gram-negative bacteria. We study the role of the bacterial shape, membrane potential and 2-D materials nature showing the interplay of these parameters in determining whether the interactions are attractive or repulsive and which one between the electrostatic and Van Der Waals forces is dominant. We calculate the interaction distances at equilibrium for different bacterial species and hydrophobic nanomaterials such as MoS2 and hydrophilic nanomaterials such as graphene oxide. A few experimental tests are reported indicating a good agreement between measurements and simulations.

Poster T4-34

Influence of crosslinking reactions of poly(benzofuran-*co*-arylacetic acid) with diamines on their thermal conductivity

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Abstract. This study reports on the preparation and thermal characterization of new polymers based on poly(benzofurane-*co*-arylacetic acid) cross-linkage reaction. The molecular structure of poly(benzofurane-*co*-arylacetic acid) offers enormous design flexibility, which allows tailoring the properties of the cured materials for a wide range of applications. The crosslinking reaction was completed by opening the lactone ring with different diamines having different reactivities. ss-^{13}C-NMR and FTIR clearly confirmed the structure of the crosslinked poly(benzofurane-*co*-arylacetic acid). The polymers, obtained as described above, have been characterized from the thermal perspective by using the photopyroeletric (PPE) calorimetry. Two dynamic thermal parameters, the thermal diffusivity and effusivity, have been directly measured using the back and front PPE detection configuration, respectively. The remaining two thermal parameters can be then calculated for a complete thermal characterization of the polymers. The static and dynamic thermal parameters determine the working temperature levels of the material, and they are essential parameters in problems involving heat transfer. **Acknowledgement**: This work was supported by a grant from the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE-2020-1595, within PNCDI III.

Poster T4-35

Plasmonic properties of metal-coated microsphere monolayers optimized for SERS applications

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Abstract. Metal-coated microsphere monolayers (MCMs) represent a class of plasmonic crystals with clearly proven capabilities as substrates for surface enhanced Raman spectroscopy (SERS). Their ability to amplify the intensities of Raman scattering of molecules by orders of magnitude relies on excitation of both localized and propagative surface plasmons. Due to their relatively easy fabrication and tunable optical response, MCMs are versatile candidates for many practical applications in the field of optical molecular sensors. Using Finite-Difference Time-Domain (FDTD) simulations, we perform a thorough analysis of the optical properties of gold-coated microsphere arrays. Specifically, we evidence the impact of sphere size, metal films thickness and fine morphology on the transmittance, reflectance and absorbance of MCMs. Furthermore, by investigating the electrical field distributions, we can link these optical properties to plasmonic effects. Finally, our results can be used to understand and optimize, through the geometry, the plasmonic properties of MCMs for SERS-based sensing. **Acknowledgement**. The research leading to this results has received funding from the NO Grants 2014-2021, under Project contract no. 32/2020.

Poster T4-36

A comparative Raman spectroscopy and XRD assessment of lattice transitions and impurities in Mn and Zn doped ferrite nanoparticles

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Abstract. Temperature-induced phase transitions and the presence of impurities to the spinel phase ferrite nanoparticles were comparatively assessed by Raman spectroscopy (RS) and X-Ray Diffraction (XRD). RS reveals gradual phase transitions from predominantly magnetite-like below 250 °C, over maghemite-like in 300-600 °C, hematite-dominated in 700-1000 °C range, and back to spinel phase at 1100 °C with different arrangement of cations on A- and B-sites than the starting sample. On the other hand, XRD on the same samples showed abrupt transition from the spinel structure to hematite between 600 and 700 °C, and back to spinel at 1100 °C, but this technique performed better at revealing other oxide phases present below the identification threshold of Raman spectroscopy. Magnetite- and maghemite-like structures in 300 to 600 °C range are more clearly distinguished by RS than XRD, due to their isostructural character (both are spinels). **Acknowledgement** This study was supported by a grant of the Romanian National Ministry of Education, CCCDI–UEFISCDI, project PN-III-P1-1.2-PCCDI-2017-0062, contract no. 58, within PNCDI III.

Poster T4-37

Functionalized SBA-3 silica: investigation of adsorption performance towards glyphosate herbicide

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Abstract. Glyphosate is a worldwide-used phosphorous herbicide. Efficient technologies are currently unavailable for glyphosate removal from waters. In this study, SBA-3 mesoporous silica-based material (amino-SBA-3) was synthesized and studied for the glyphosate removal from water. The obtained silica material was characterized by SEM, TG, FTIR, BET surface area and pore size distribution measurements. In order to elucidate specific interactions between the mesoporous silica and glyphosate via phosphoric group, a surface functionalization with (3-aminopropyl)triethoxysilane was accomplished. The performance observed for the mesoporous silica material (quantitative adsorption and complete recovery of silica) is worth of note, mostly considering that the sorbent can be regenerated and reused with unaltered performances for at least five cycles. **Acknowledgements**: The work has been funded by the Romanian Ministry of Research, Innovation and Digitalization, NUCLEU Program-Financing Contract no. 9N/2019, under Project PN 19 11 03 01 “Studies on the obtaining and improvement of the acido-basic properties of the nanoporous catalytic materials for application in wastes valorization”.

Poster T4-38

$CoFe_2O_4$ /TiO_2:Tb nanoparticles as an emerging magnetic photocatalyst

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Abstract. The $CoFe_2O_4$/TiO_2:Tb composite nanoparticles were prepared by a two-stage chemical route. The composites were characterized by using X-Ray Diffraction, Transmission Electron Microscopy, X-ray and UV Photoelectron Spectroscopies, FT-IR, Raman and UV-Vis spectroscopies. There is a polarized spin transfer at the interface between the cobalt ferrite into the TiO_2 conduction band. As a result the magnetic moments of oxygen vacancies in TiO_2 becomes (ferro) magnetically ordered. The magnetic moments sublattice of Tb ions may have an either “ferro” or “antifero” coupling depending on the dopant concentration. The magnetic semiconductor intensifies the optical absorption in the visible. There is a band-to-band absorption assisted by single-occupied oxygen vacancies coupled to some local crystal lattice relaxations. The lifetime of the photoexcited electrons in the conduction band increases due to their coupling with magnetically ordered interface transferred states. Also the trapping of electrons into multiplet states of Tb^{3+} reduces the recombination rate. The photocatalytic efficiency of the magnetically ordered titania increases with respect to bare TiO_2. The reactive oxygen species produced at the solid–liquid interface of TiO_2 were identified by Electron Spin Resonance coupled with spin-trapping technique. The results were correlated to the presence of the magnetic order inside the titania.

Poster T4-39

Structural assessment of silica and amino-functionalized silica nanoparticles by FTIR and Raman Spectroscopy

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Abstract. Mesoporous silica nanoparticles were synthesised by sol-gel method using cetyltrimethylamonium bromide (CTAB) micelles as template and the same method was used for amino-silica nanoparticles synthesis. Compositional and structural analysis of materials involved FTIR and Raman spectroscopic study. A comparative study of the spectra revealed the distinctive pattern for the observed samples, such as a strong peak at 1030-1050cm^{-1} in the FTIR spectra, characteristic for Si-O-Si stretching vibration or the specific pattern of silica between 90-500 cm^{-1} and 2880-2980 cm^{-1}, in the Raman spectra. A point of interest in this study was the control of CTAB removal during the second stage of synthesis. This was highlighted in the FTIR spectra by decreasing in intensity or disappearance of the peaks 2850 and 2930 cm^{-1} due to absorption of -CH_2- groups. The presence of –NH_2- in the amino-silica was highlighted by the changes in the region 1000-1500 cm^{-1} in the Raman spectra. The two spectroscopic methods offer valuable information for structural characterization of silica nanoparticles.

Poster T4-40

Electrochemical detection of His-Tagged CA19-9 Antigen with triple-doped graphene modified electrode

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Abstract. His tag CA19–9 (Carbohydrate antigen N-terminal His Tag) is a typical biomarker for gastrointestinal cancer tumors and represents a highly sialylated glycoprotein showing 85% carbohydrate by weight, that attaches to O-glycans on the surface of cells and plays a vital role in the cell-to-cell recognition processes. Two graphene-based materials were prepared by exfoliation of graphite rod with pulses of current. The first material (denoted EGr-1) was exfoliated in a mixture of ammonium sulfate, boric acid and sodium chloride (1:1:1 ratios). The second material (denoted EGr-2) was prepared by exfoliation of the graphite rod in a mixture of ammonium sulfate, boric acid and sodium chloride (0.5:1:0.5 ratios). Both materials were morphologically and structurally characterized by FTIR, XRD, and SEM. After preparation, the materials were used for the modification of two glassy carbon electrodes, denoted GC/EGr-1 and GC/EGr-2, respectively and used for electrochemical detection. **Acknowledgement**: This work was supported by grants of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCCF-2016-0006, and project number 500PED/2021, within PNCDI III.

Poster T4-41

Hybrid PVDF-P(L-DOPA)-ZnO membranes for efficient pollutants removal

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Abstract. Membrane filtration is one of the most promising technologies for the treatment of wastewater due to the easy operation, energy saving and high separation efficiency. But the hydrophobic nature of the membrane drives to organic pollutants adsorption on its surface resulting on a severe fouling. One solution to solve this issue is to use nanoparticles with photocatalytic activity to modify the membrane surface. PVDF-P(L-DOPA)-ZnO hybrid membranes were prepared and tested against two classes of water pollutants: cationic dyes and antibiotics. The structural and morphological properties of the hybrid membranes were evaluated by X-Ray diffraction (XRD), Attenuated Total Reflection- Fourier Transform Infrared Spectroscopy (ATR-FTIR), Scanning Electron Microscopy (SEM). The firm P(L-DOPA)-ZnO coating on PVDF membrane surface converted its hydrophobic nature to a hydrophilic one. Under UV light irradiation of PVDF-P(L-DOPA)-ZnO hybrid membranes, the removal rate for Rhodamine B (RhB) and oxytetracycline (OTC) reached 80% and 71%, respectively. The hybrid membrane is characterized by a high stability and reusability in the process of dye removal. The generation of reactive oxygen species involved in photocatalysis was proved by ESR. **Acknowledgments**. This work was supported by the Ministry of Research, Innovation and Digitization - MCID, Competitiveness Operational Programme, POC Project 18/01.09.16, SMIS Code 105533.

Poster T4-42

Charge-Transfer Resistance in Nitrogen-Doped Graphene

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Abstract. Nitrogen-doped graphene samples were synthesized by the hydrothermal method at 160^{o} C for 3, 8 and 12 hours. The samples were correspondingly denoted NGr-1, NGr-2 and NGr-3. Their morphology, structure and electrochemical properties were investigated by SEM/TEM, X-ray powder diffraction (XRD), elemental analysis, Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS). For NGr-1 and NGr-2 samples, the elemental analysis indicated a nitrogen concentration of around 6.36 wt% whereas in the case of NGr-3 sample the concentration was slightly higher (6.85 wt%). The electrochemical studies performed with NGr modified electrodes proved that the charge-transfer resistance (R_{ct}) depends not only on the nitrogen doping level but also on the type of nitrogen atoms found at the surface (pyrrolic-N, pyridinic-N, graphitic-N). **Acknowledgement:** *This work was supported by grants of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number* PN-III-P4-ID-PCCF-2016-0006 and project 500PED/2021*, within PNCDI III.*

Poster T4-43

Reducing, recycling and reusing of construction and demolition wastes by the incorporation in the glasses

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Abstract. Construction and demolition wastes occupy to the large storage spaces and cause pollution. Until now, the obtaining of the new products such as concrete and bricks was limited to the addition of suitable binders contents, compaction and heat treatment, without to exist a concrete recycling method. In this paper, ten types of composites were prepared by an eco-inovative method including the following wastes in the crushed glasses: brick, autoclaved aerated concrete, plaster, mortar, lead, lime, iron (with varied contents), cast iron, ash. The prepared materials were characterized by the analysis of XRD and SEM, IR and UV-Vis spectroscopy. Our results show structural modifications in the silicate network, the processes of water absorption and electronic transitions of metalic ions. The composites can be used in the concrete industry with high quality due the presence of cristalline phases originated from waste with role in the water absorption process.

Poster T4-44

TiO_2 nanotubes/graphene/metal nanoparticles as suitable photocatalyst for degradation of ciprofloxacine as an emerging pollutant

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Abstract. Ternary nanostructures of TiO_2 nanotubes/graphene/metal nanoparticles were successfully synthesized *via* chemical and thermal treatment methods. The photocatalytic ability of resulting ternary nanostructures was investigated on degradation of ciprofloxacine (fluoroquinolone antibiotic) that is frequently detected in aquatic environments. Photocatalytic experiments were performed in a Photoreactor Luzchem LZC-4V using UV and visible light as source of irradiation. Spectroscopic/analytical methods were used to evaluate the photocatalytic processes of ciprofloxacine degradation and also, the kinetics of reaction was analyzed. Findings from this study further expand the spectrum of emerging pollutants removal from aquatic systems under photocatalytic conditions.
Acknowledgments. The research leading to these results has received funding from the Norwegian Financial Mechanism 2014 -2021, under Project RO-NO-0616, contract no. 29/2020.

Poster T4-45

Structural changes in nanostructured silica core-alumina shell microspheres doped with iron and gadolinium investigated by Solid-State NMR Spectroscopy

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Abstract. We report new nanostructured silica core-alumina shell microspheres doped with paramagnetic ions, obtained by a chemical synthesis based on Stöber method for the silica core, and electrostatic attraction for nucleation of shell. Amorphous character of the structures was highlighted by XRD. Structural changes that occur in samples by changing the concentration of paramagnetic ions from the shell are studied by solid-state NMR. Shape and size of microspheres were investigated by TEM. The results show that the paramagnetic ions have a disordering effect, partially substituting aluminium, which was incorporated in silica network. We have obtained stable amorphous microspheres with highly porous shell, and paramagnetic ions on the outermost layer of the structures, having potential application as contrast agents in magnetic resonance imaging.

Poster T4-46

Surface interaction studies of novel 2D materials with gram-negative and gram-positive pathogens and an enveloped virus

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Abstract. The intriguing interactions of the most studied two dimensional nanomaterials with live matter such as bacteria and viruses form a base to understand the surface phenomena of nano-macro objects. The novel physico-chemical properties of 2D materials are the driving force to exhibit their anti-bacterial and anti-viral actions. In the current study, an extensive study was carried out between a gram-negative (Escherichia coli), and a gram-positive (Staphylococcus aureus) bacterium with two different 2D materials such as MoS_2 and graphene oxide nanosheets exfoliated in water only. Also, the same 2D materials were utilized to study their anti-viral action with Herpes simplex virus type-1, (HSV-1). The two 2D materials behaved differently with the given bacteria and virus with very interesting results. A very simple Derjaguin–Landau– Verwey–Overbeek theory was employed to form the base to interpret the antibacterial action of the given 2D materials. Morphological results showed strong mechanical damage to the bacteria by MoS_2 nanosheets. On the other side, graphene oxide showed very surprising results exhibiting strong anti-viral action than MoS_2. Another part of the study reveals very preliminary results on the anti-bacterial action of graphene nanosheets exfoliated in Cyrene showing the toxicity behavior of the material.

Poster T4-47

Evaluation of graphene on the photocatalytic properties of copper oxides/graphene composites compared to copper oxides/graphene/TiO_2 composites

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Abstract. A series of copper oxides-titanium dioxide-reduced graphene oxide (CuO/Cu_2O/rGO) composites were prepared vi a simple procedure starting from copper nitrate, TiO_2 nanoparticles and/or graphene oxide. These composites possess different copper ratio (1, 2 or 3 %) and different reduction degrees for graphene, and were completely characterized in terms of morphology and spectroscopical aspects. Their physico-chemical properties (powder X-ray diffraction, XPS spectroscopy, diffuse reflectance UV-Vis and IR spectroscopy), the oxidation degree of the copper atoms and reduction degree of the graphene were correlated with their photocatalytic activity by measuring the rate of methylene blue (MB) degradation under UV and visible light. MB was selected because of its strong adsorption to metal oxide surfaces, well defined optical absorption and good resistance to light degradation. **Acknowledgement:** "The research leading to these results has received funding from the Norwegian Financial Mechanism 2014 -2021, under Project RO-NO-0616, contract no. 29/2020"

Poster T4-48

Application of nanocomposites based on CNT-COOH as adsorbents for the removal of tartrazine from aqueous solutions

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Abstract. Many industrial processes use a variety of synthetic chemical dyes (e.g. the industry of paper, textiles, printing etc). It has been estimated that approximatively 50% of synthetic dyes annually produced, are azo dyes very resistant to light, temperature and oxidizers. These are non-degradable and causes bioaccumulation in living organisms. For this reason, a great attention has been focused on the elimination of the dyes from effluents, due to their potential toxicity. Various methods for dye removal are adopted and the adsorption has been reported to be the most effective method that provides promising relevant results. The magnetic nanocomposites based on carbon nanotubes (CNT) are among the adsorbent materials with promising properties. The present investigations concern the application of magnetic nanocomposites CNT-COOH/Fe_3O_4 and CNT-COOH/Fe_3O_4/NiO as adsorbents for the removal of tartrazine, a hazardous dye, from aqueous solutions. In order to establish the conditions for optimal retention of tartrazine, the influence of initial pH of the dye solution, temperature, adsorbent dose, contact time and the initial concentration of dye was evaluated. **Acknowledgments:** This work was carried out through the Romanian Ministry of Research, Innovation and Digitization within the Core Program, PN19-35-0203 (36N/13.02.2019).

Poster T4-49

Magnetic Properties of $Nd_2Fe_{14}B$/Fe Exchange Coupled Nanocomposite Nanoparticles obtained by Matrix Milling and Annealing

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Abstract. In this work, we have produced $Nd_2Fe_{14}B$+Fe exchange-coupled nanocomposite nanoparticles trough matrix milling. $Nd_2Fe_{14}B$ and Fe powders were first milled for 6 h in a planetary ball mill, the resulting composite powders was mixed in a 60:1 weight ratio with CaO_2 powder, this mixture was then milled for a further 6 h. The nanocomposite powder was then annealed while still in the CaO_2 matrix. After annealing the matrix was chemically dissolved leaving behing only the nanocomposite powder. Once separated from the matrix, the structure of the nanocomposite was studied by X-Ray diffraction, the magnetic properties of the materials were studied by measuring demagnetization curves up to 10 T and the particles morphology and chemical homogeneity were stuied by scanning electron microscopy and X-ray microanalysis (EDX). **Acknowledgement:** Financial support of Romanian Ministry of Research, Innovation and Digitalization, grant PN-III-P2-2.1-PED-2019-4696.

Poster T4-50

Synthesis and characterization of nickel oxide-silver-antibiotic nanocomposites

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Combination of nanotechnology and traditional antibiotic has been adopted as a promising tool to solve the problem raised by the antimicrobial resistance in the treatment of bacterial infectious diseases. Extensive research studies have revealed improved activity of nanoparticles when used in combination with antibiotics against various pathogenic microorganisms. Silver nanoparticles (Ag NPs) in combination with antibiotics have also been shown to exhibit significant antimicrobial activity and reduced toxic effect. Likewise, previous studies have demonstrated the effectiveness of nickel oxide nanoparticles (NiO NPs) against gram-positive and gram-negative pathogenic bacteria, and moreover, their low toxicity and good biocompatibility. In this work, NiO-Ag-antibiotic composite materials (antibiotic: sulfamethoxazole, norfloxacin) were successfully prepared and further characterized by using several techniques such as X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), scanning electron microscopy (SEM), UV-Vis spectroscopy. The effect of calcination temperature on the crystallinity, morphology and size of NiO NPs was investigated. **Acknowledgements**: Financial support from the Romanian Ministry of Research, Innovation and Digitalization (MCID), Core Programme, Project PN19-35 02 03 is gratefully acknowledged.

Poster T4-51

Insights into the photocatalytic activity of g-C_3N_4-TiO_2:Cu nanocomposites

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Abstract. In modern society, nanomaterials are showing great potential for enabling and improving technologies for water treatment by photocatalysis. In photocatalytic processes reactive oxygen species (ROS) play crucial roles in the degradation of most organic compounds (dyes, antibiotics, etc) in the solution. g-C_3N_4-TiO_2 nanocomposites has attracted much attention due to its functionalities combining the properties of TiO_2 and graphitic carbon nitride (g-C_3N_4) in one single entity. The present work is focused on the photocatalytic properties of g-C_3N_4-TiO_2:Cu nanocomposites obtained by deposition of TiO_2:Cu nanoparticles obtained through a sol-gel process onto the g-C_3N_4 resulted from decomposition of urea. X-ray diffraction (XRD), transmission electron microscopy (TEM) and high resolution (HRTEM), thermogravimetric analysis (TGA), UV-vis diffuse reflectance spectroscopy (DRS), surface area and porosity measurements were used to characterize the obtained nanocomposites. The photocatalytic activity toward the degradation of RhB solution, under visible light irradiation was performed. Additionally, the electron spin resonance spectroscopy (EPR) coupled with spin trapping technique was performed to evidence the generation of ROS during irradiation, capable to degrade the organic molecules of RhB. **Acknowledgements.** This work was supported by the Romanian Ministry of Research, Innovation and Digitization, Core Programme, Project PN19 35 02 03

Poster T4-52

Synthesis and characterization of Fe_3O_4/MnO_2 nanocomposite for improving of biodiesel production

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Abstract. Biodiesel production is becoming more and more important in the last years and different methods for production are tested. Thus, biodiesel can be obtained from different vegetable oils or animal fats using catalysts. The aim of this research was to prepare the Fe_3O_4/MnO_2 nanocomposite and test them as catalyst to obtain biofuel from seeds and grapes oil. The transesterification in microwave field was used for biofuel obtaining. Fe_3O_4/MnO_2 nanocomposite was synthesized by chemically and biochemically (using plant extracts) routes and characterized regarding size, crystallinity, composition, porosity and specific surface area. The analysis of the final results revealed that the samples prepared by chemically procedure have smaller sizes, specific surface area higher than the samples prepared using plant extract. The Fe_3O_4/MnO_2 nanocomposite with the highest specific surface area from all prepared nanocomposites was tested as catalyst for microwave-assisted transesterification studies. This determined an increasing reaction rate of the transesterification process, being a promising route for biodiesel production. **Acknowledgments:** This work was carried out through the Romanian Ministry of Research, Innovation and Digitization within the Core Program, PN19-35-0203 (36N/13.02.2019).

Poster T4-53

Mesoporous silica materials: investigation of catalytic performance towards chlorinated pesticides

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Abstract. Chlorinated hydrocarbons are intensively used as solvents or raw materials for the synthesis of various products, such as pesticides, cleaning agents or and poly vinyl chloride (PVC). However, they cause serious environmental problems when they are released into water. Catalytic degradation of chlorinated hydrocarbons is considered as a promising process, resulting potential useful chemicals, such as hydrocarbons or HC1. In this study, mesoporous SBA-15-type silica, was synthesized using a sol-gel method. In order to load a metal on the support, SBA-15 was silanized with APTES, followed by impregnation with nickel acetate solution. Degradation reaction kinetics of the prepared catalysts was investigated using Aldrin and DDT as model systems. Reaction products were sampled at the outlet of the reactor and analysed by gas-chromatography. This study demonstrates the potential of a simple and efficient approach for the removal of organochlorine pesticides from waters.**Acknowledgements**: The work has been funded by the Romanian Ministry of Research, Innovation and Digitalization, NUCLEU Program-Financing Contract no. 9N/2019, under Project PN 19 11 03 01 "Studies on the obtaining and improvement of the acido-basic properties of the nanoporous catalytic materials for application in wastes valorisation".

Poster T4-54

Multi-walled carbon nanotubes decored with Ag / TiO_2 nanoparticles

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Abstract . Multi-walled carbon nanotubes (MWCNT) were coated Ag doped TiO_2 via Pechini method using mixture of 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. The structure of Ag:TiO_2/MWCNT samples (note 0.5% Ag, 1.0% Ag, 1.5% Ag, 2.0% Ag and 2.5% Ag related to the Ag^+/Ti^{4+} atomic radio), was determined by Bruker D8 Advanced diffractometer with CuKα radiation. XRD analysis revealed the formation of CNT, TiO_2 (anatase and rutile) and Ag. Their morphology and sizes were investigated with scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM with EDX), which shows that nanoparticles were coated on MWCNT. The UV – VIS absorption results indicated interaction between TiO_2 and CNTs, the composite material can absorb at higer wavelength. In Raman spectra the characteristic vibration of the TiO_2, Ag and C atoms of graphite are identified. The photocatalytic activity of the Ag:TiO_2/MWCNT was assessed by examining the degradation of Allura red (E129) from model aqueous solutions as a probe reaction under visible light and ultrasonic irradiation. The efficiency of catalysts on Allura Red degradation reached high values above 70% for 2.0%Ag. The dye photodegradation process follows a pseudo – first – order kinetic with respect to the Langmuir – Hinshelwood reaction mechanism. **Acknowledgement***:* This research was financially supported by the MEC, Nucleu – Program, project PN19 35 02 03.

Poster T4-55

GNP-based sandwich immunosensor for SERS biomarker detection in liquid

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Abstract. Gold nanoparticle (GNP)-based immunosensors represent a class of promising sensing tools. By combining the capability for biofunctionalisation with the exceptional properties of GNPs, sensitive detection of bio-relevant molecules can be rapidly and cost-effectively achieved. Herein we propose a Surface Enhanced Raman Scattering (SERS) immunosensor for detecting and quantifying model biomarker proteins. Spherical (GNSs) and urchin-like (GNUs) gold nanoparticles were spectroscopically labelled, PEG-coated, and functionalized with capturing antibodies. In the presence of the target antigen, GNP pairs are formed and the amplification of the label molecule signal is observed *via* hot-spots formation in interparticle gaps. Two different sensing configurations: pairs of GNUs-GNUs and GNUs-GNSs were experimentally tested and theoretically modelled by FDTD. Tracking down small analyte concentrations *via* SERS with an easy-to-handle, portable Raman device in tandem with the capacity for in-liquid detection makes the proposed system feasible as a point-of-care assay. **Acknowledgement**: Entrepreneurship for innovation through doctoral and postdoctoral research, POCU/380/6/13/ 123886 co-financed by the European Social Fund, through the Operational Program for Human Capital 2014-2020.

Poster T4-56

Effect of the Mn amount on the photocatalytic activity of Mn doped TiO_2-MWCNT nanocomposites

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Abstract. A series of Mn doped TiO_2-MWCNT nanocomposites was prepared by a polymer wrapping-technique. In the first stage, Mn doped TiO_2 nanoparticles were synthesized by sol-gel method, and then, the obtained nanoparticles were attached on functionalized MWCNT. MWCNT and TiO_2 crystalline phases were evidenced using XRD. The specific bands of MWCNT and TiO_2 components were highlighted by FT-IR spectroscopy. The presence of Mn^{2+} and Mn^{4+} ions were probed by EPR and XPS spectroscopies. TEM images provided evidence of the attaching and distribution along the nanotubes of Mn doped TiO_2 nanoparticles with spherical form. The energy band gap of nanocomposites decreased with the increase of manganese amount. Evaluation of nanocomposites as photocatalysts for degradation of RhB dye solutions under UV irradiation demonstrated that sample containing 0.5% Mn shows the best photocatalytic performance. The mechanism of photocatalytic activity was elucidated based on the reactive oxygen species involved in this process. **Acknowledgements.** This work was supported by the Romanian Ministry of Research, Innovation and Digitization, Core Programme, Project PN19 35 02 03.

Poster T4-57

Evaluation of N-doped graphene role in the photodegradation of sulfamethoxazole

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Sulfamethoxazole is an emerging contaminant that is found in surface waters. In this study we followed its removal by means of adsorption and photocatalysis processes using materials based on N-doped graphene/TiO_2. These processes were monitored using liquid chromatography (HPLC, on a C18 column). The photocatalytic activity of the prepared materials was performed under UVA light (320-400 nm) and cold white light (420 – 800 nm) using a Luzchem LZC-4V photoreactor. The experimental results demonstrated the photocatalytic performance of the TiO_2Ag-N-doped graphene in correlation with the experimental results obtained from the physico-chemical properties (XPS VB spectroscopy and diffuse reflectance UV-Vis measurements). **Acknowledgments**: The financial support for this work was provided by the Romanian Ministry of Research and Innovation, program Nucleu, contract no. PN 19 35 02 02/2019.

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Electrochemical detection of 8-Hydroxy-2'-Deoxyguanosine biomarker with new graphene modified carbon electrode

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Abstract. 8-Hydroxy-2'-Deoxyguanosine Biomarker (8-OH-dG) is a cancer biomarker for tumors and it is used for the evaluation of oxidative damage processes in DNA. Graphite exfoliation with pulses of current has a lot of advantages for the graphene synthesis. In this work we prepared two graphene-based materials doped with nitrogen, sulfur and boron in different proportions, following denoted EXF-1, and EXF-2. Both materials were morphologically and structurally characterized by SEM, FTIR, and XRD and they were used for the modification of two glassy carbon electrodes, denoted GC/EXF-1 and GC/EXF-2. The electrochemical performances obtained for the 8-OH-dG detection with these new graphene-modified electrodes are very good and promising for real sample analysis. **Acknowledgement:** This work was supported by grants of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCCF-2016-0006, within PNCDI III.

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