14th International Conference

PROCESSES IN ISOTOPES AND MOLECULES

Cluj-Napoca, 2023

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Welcome at PIM 2023

It is a pleasure for the National Institute for Research and Development of Isotopic and Molecular Technologies to host the 14th 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 2023 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.

Topics:

T1 – Stable Isotopes and Emerging Approaches

T2 – Molecules, Biomolecules and Photonics

T3 – Green Energy and Innovative Technologies

T4 – Nanostructured 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

Advancements in compound-specific analysis for the verification of food authenticity

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Abstract. Stable isotope ratio analysis has been used for food authenticity testing for more than thirty years and is now used on a routine basis for a wide variety of food products. Recently, important developments have been made in the analytical method and the understanding of fractionation processes resulting in isotope differences suitable for food authentication has been improved. However, bulk stable isotope value represents an average value of all components in a food product and, in some cases, may not sufficiently distinguish isotopic variations between different samples. Compared to bulk samples, more isotopic information can be obtained by focusing on the isotopic composition of specific food compounds. Compound Specific Isotope Analysis can be based on both offline and online compound isolation prior to isotope analysis. In-line systems are accomplished by combining a gas chromatograph (GC) or liquid chromatograph (LC) separating individual compounds in a complex mixture, connected to an isotope ratio mass spectrometer (IRMS), resulting in the stable isotope ratios of specific compounds in the samples. Combined food authentication applications based on GC-IRMS and LC-IRMS have grown significantly in recent years mainly focused on synthetic versus natural compounds and traceability according to agricultural practices and geographical origin.

Plenary Pl-2

Solid-State NMR of Pharmaceuticals and Plant Cell Walls

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Abstract. Solid-State magic-angle spinning (MAS) NMR is a valuable tool in the characterisation and study of active pharmaceutical ingredients (APIs). Heteronuclear ^{1}H-^{13}C correlation experiments are invaluable for assignment, while homonuclear ^{1}H-^{1}H double-quantum (DQ) single-quantum (SQ) experiments reveal proximities (typically under 3.5 Angstroms) among pairs of hydrogen atoms. In addition, ^{14}N-^{1}H spectra show one-bond NH connectivities or additionally longer-range NH proximities depending on the recoupling time employed. In the emerging NMR crystallography concept (recognized as a sub area by the International Union for Crystallography and, in the UK, by funding for a collaborative computational program for NMR crystallography, www.ccpnc.ac.uk), experimental solid-state NMR is complemented by first-principles calculations of NMR parameters using the GIPAW (gauge-including projector augmented wave) density-functional theory planewave approach that is particularly suited to periodic solids. In addition, the talk presents the application of ^{13}C-^{13}C refocused INADEQUATE DQ-SQ to plant cell walls incorporating ^{13}C labelling].

Plenary Pl-3

Identification of point defects via EPR spectroscopy and elucidating their roles in supercapacitor devices

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Electron paramagnetic resonance (EPR) spectroscopy is a very powerful method due to its enhanced sensitivity to unpaired electrons. In order to understand the defect structure in functional nano-materials we use multi-frequency EPR spectroscopy. In this presentation i) basics of EPR spectroscopy, ii) quantum confinement effects in ferroelectric nano-materials and iii) EPR and Photoluminescence (PL) investigations of intrinsic defect centers in semiconductor zinc oxide (ZnO) nanoparticles will be given. Starting with the introductory information about EPR spectroscopy; doping and nano-size effects will be discussed for the ferroelectric materials such as, $PbTiO_3$, $BaTiO_3$, $PbZrTiO_3$ (PZT) etc. In the last part of the talk, surface and core defects and their reactivity under temperature and light will be presented for ZnO semiconductor nano-materials. Defect models will be discussed. Finally application of such materials as electrode materials and their electrochemical performance test results in the supercapacitor devices will be presented.

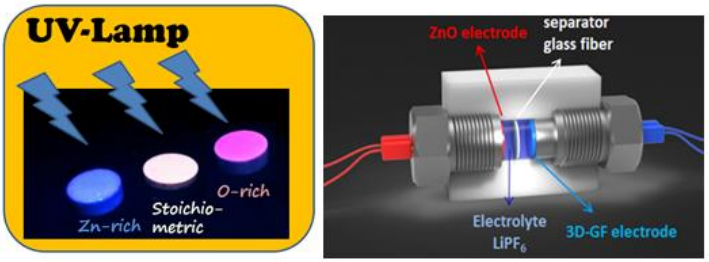

Figure: (left) Defect evolution of non-stoichiometric ZnO. (right) The supercapacitor device based on ZnO and 3D graphene foam electrodes.

Plenary Pl-4

Functional nanostructured materials: A biophysical insights for molecular detection and delivery systems

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Abstract. The development of innovative molecular detection and delivery platforms is important for both compounds of interest in medicine, and in monitoring the environment or food quality. Nanotechnology is increasingly used, and nanomaterials can be tailored to obtain nanostructured functional materials for the development of both molecular sensing and molecular delivery systems. Nanomaterials can be used as electrical conduction amplifier, signal amplifier or biomolecular recognition component, but also as nano-carriers for molecules.

In this talk we will highlight the use of nanomaterials and nanocomposites, both commercially available and synthesized in our laboratory. The functional nanostructured materials obtained used for the development of molecular detection and delivery systems were characterized and their interaction with the molecules of interest was evaluated through a biophysical approach.

Thus, it was aimed to obtain an increased selectivity facilitating the applicability of our molecular sensing in the analysis of real samples and obtaining diagnosis at the point of care (POC) or Point-of-need (PON). For our molecular delivery systems, an efficient approach for molecular delivery was ascertained in different applications.

Plenary Pl-5

Stable isotopes and chemometrics in food authentication: applications in antifraud laboratories.

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Abstract. The control of food authenticity is of major importance to protect European consumers and trades who valorise some production through protected denominations that define strict rules of production, quality, and specific geographic localization of production. The role of food control laboratories is to determine the compliance between the commodity and the label allegations. In order to detect adulterations and wrong geographical origins, stable isotope and mineral concentration are, among other analytical parameters, very powerful tools. Moreover, due to fast commercial exchanges, it is also necessary to develop fast analysis based on rapid analytical techniques not requesting long preparation or are designed for in situ measurements. These analyses require authentic samples to elaborate statistical models with the help of chemometric tools. Various examples and their applications, developed in the French antifraud laboratories net, will be presented to illustrate various applications like stable isotope analyses to control the origin of bubbles in sparkling beverages, the geographical origin of fish, and the application of Lead isotope ratio to determine wine origin. Then 1H NMR and IR signals data treatment will be emphasized to illustrate the application of chemometrics in the control of honey authenticity.

Plenary Pl-6

Experimental study of stratospheric vortices generated by wildfires

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Abstract. Wildfires, such as the Australian 2019-2020 wildfires, generate plumes that deposit large quantities of smoke in the stratosphere, comparable to a moderate volcanic eruption. These smoke plumes self-organise as synoptic scale anticyclonic vortices that rise due to the internal heating generated by the absorption of solar radiation on the black carbon particles. These structures persist for several months in the stratosphere, rise by 10 to 20 km and travel over considerable distances. Such phenomenon has never been detected and described in the literature before. We aim to understand by means of laboratory experiments the processes under which a smoke plume can spontaneously organise into a persistent vortex. I will present the first experimental results on the dynamics of a vortex obtained by injecting a buoyancy source in a stratified fluid placed on a turning table.

Plenary Pl-7

Nano-structured materials for catalytic applications

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Abstract. The role of catalysis is fundamental for the chemical production especially in recent years in which the development of increasingly sophisticated catalysts is mandatory to meet the needs of sustainable development. Nano-structured materials represent a family of potential candidates to answer the requests of market. In this field, the research is moving in two parallel directions: i) the substitution of obsolete processes with more environmentally sustainable ones; ii) the production of new building blocks and products from renewable sources. Nanomaterials have proven to be highly effective for a large number of classes of reactions and for this reason numerous techniques have been developed for the realization of nanoparticles for the formulation of active and selective catalysts. The characterization and study of reaction mechanisms helps more the understanding of the structure/properties relationship which make it possible to obtain more performing phases. Nowadays it is appropriate that the research focuses its efforts not only on finding the most suitable material for a chemical transformation but also on the parameters that regulate its synthetic procedure. In fact, the realization of nanostructured catalysts often requires many steps that are often difficult to control and difficult to scale-up at industrial level. Trying to modify the synthetic pathways to obtain nanostructured materials with similar characteristics, perhaps one-pot, in many cases is still very challenging. For example, the production of hydrogen starting from CO_2 rich mixtures requires catalysts in which the key role is played by the size of the active phase nanoparticles, which can be obtained by single-step wet aqueous synthesis procedures, reducing the amount of solvents and the number of unit operations.

Plenary Pl-8

Femtosecond Laser Micromachining for Lab on a Chip Applications

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Abstract. Since the first pioneering works in the late nineties that demonstrated modifications induced in a transparent material by focusing a sub-picosecond pulse, femtosecond laser micromachining have been widely used in many research applications ranging from material processing to micro-devices' fabrication. Indeed, the strong versatility of femtosecond laser micromachining of transparent materials like glass, allows to induce permanent refractive index modifications in the bulk of substrates, to selective remove material to create microfluidic networks or even to create three-dimensional free-standing structures by direct laser writing.

Plenary Pl-9

Functional and structural characterization of Bone Morphogenetic Protein 2 and the antagonist Noggin

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Abstract. Bone morphogenetic proteins (BMPs) belongs to the transforming growth factor-β superfamily of multifunctional cytokines. The findings that they induce a wide range of different cellular effects have opened stimulating opportunities towards new therapeutic approaches for the treatment of many diseases and/or metabolic disorders. Thus, BMP-2 and BMP-7 have been approved by the FDA for clinical application in the context of bone repair. However, the lack of knowledge concerning BMP interaction pathways has been responsible for a misunderstanding and an underappreciation of the side effects associated with BMP-based therapeutic approaches. Therefore, the high degree of interest in BMPs as potential biopharmaceuticals is now mitigated by some unresolved issues.

In this study, we used BMP-2 as a model system to gain insight into both the relationship between structure and function in BMPs and the principles that govern affinity for their cognate antagonist Noggin. Both proteins were produced and characterized with the help of complementary biophysical techniques, including optical spectroscopies, mass spectrometry, multi-angle light scattering coupled with size exclusion chromatography, and X-ray crystallography. Furthermore, a series of *in vitro* cell-based assays were performed, in combination with enzymatic measurements, RT-qPCR and matrix staining, which allowed monitoring of differentiation.

Plenary Pl-10

Polar polymers in actuators, sensors, and generators

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Abstract. High dielectric permittivity polymers are an important material class that may be applied in actuators, sensors, and energy harvesting and storage. Their glass transition temperature (T_g) can be tuned at will by the type and content of the polar groups used and the polymer backbone on which they are grafted. Proper cross-linking of the low T_g polymers allowed us to achieve a novel class of polar elastomers with unique dielectric properties. In contrast, poled high T_g polymer nanoparticles in an elastic network allow for achieving piezoelectric elastomers. These novel materials are used as dielectrics in elastic capacitors, which can serve as actuators, sensors, or generators.

This presentation will show the synthesis of polar polymers, their processing into thin elastic films, and their use in different applications.

Acknowledgments. We gratefully acknowledge the financial support from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 101001182), and Swiss National Science Foundation (206021_150638/1), EU Marie Curie ITN project SMART (860108), and Swiss Federal Laboratories for Materials Science and Technology (Empa).

Plenary Pl-11

Optimization of ^{13}C enrichment by carbon monoxide cryogenic distillation

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Abstract. In this work, the cryogenic distillation of carbon monoxide (CO) is discussed in order to obtain an isotopic enrichment in ^{13}CO, considering the importance it assumes due to its successful use in medical research and other fields. In particular, it deals with the simulation of CO cryogenic distillation for enrichment in ^{13}CO with the aim of: (i) evaluating and optimizing the performances of the semi-batch operating mode, and (ii) building up a useful model that may be exploited to optimize column operation during time-depending runs without the need for too expensive experimental campaigns. To pursue these goals, established methods well known in the field of chemical and process engineering have been used and a commercially available software has been employed both for process simulation and design, after validation against experimental data from the pilot distillation packed column of the National Institute for Research and Development of Isotopic and Molecular Technologies (INCDTIM). The good agreement between the experimental data and the simulation results proved the reliability of the model, then used to analyse the impact of operating variables on column performances and to develop an improved cycle for future optimized runs.

Plenary Pl-12

Climate change or banning herbicides will not let our glass empty! Insights from molecules and isotopes

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Abstract. The grapevine is one of the most-important edible fruit-plants cultivated worldwide. The level of grapevine-weed competition for water and nitrogen was assessed by comparing field, chemical, molecular and isotopic measurements. The data set included the $d^{13}C$ values of must sugars, concentrations and $d^{13}C$ of leaf epicuticular lipids, and $d^{13}C$ and $d^{15}N$ of wine volatile compounds and solid residues. Samples come from field-experiments combining irrigations and soil-management practices, various cultivars, and growing seasons. The molecular and isotopic values varied strongly with soil water availability and management. The vine-weed competition for nitrogen is exacerbated in water-deficient vines. These molecular and isotopic data showed a better resolution and separation of the vine groups from different soil management practices and irrigation treatments compared to the field-measurements. The red grapevines adapt much better than white grapevines to soil water and nitrogen deficits. White grapevines must be well watered to avoid deficient uptake of soil nitrogen. Drip irrigation is not a sustainable solution, but as an agroecological solution, minimal and efficient irrigation (with rain, lake, or river water) will decrease the dose of applied herbicides. This action will alleviate the pressure on winegrowers regarding the time needed to develop a sustainable nonchemical soil management.

Plenary Pl-13

New results in the development proton exchange membrane fuel cell components

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Abstract. Polymer electrolyte membrane fuel cells (PEMFCs) convert chemical energy into electricity in an efficient and environmentally friendly way. Electrocatalysts are the primary elements of PEMFCs. The most commonly used commercial PEMFCs electrocatalyst, the carbon supported platinum (Pt/C), is known to suffer from electrocorrosion and is not resistant to CO poisoning. In $Ti_{(1-x)}M_xO_2$-C (M: Mo, Sn; x: 0.1-0.3) multifunctional supports the carbon backbone is responsible for the high surface area and electrical conductivity, the TiO_2 component helps in stabilizing the Pt in highly dispersed state thus offering resistance against electrocorrosion, and the dopant M provides important co-catalytic function via the bifunctional mechanism while remains protected against dissolution by the TiO_2 matrix. In this contribution, our efforts were aimed at elucidating the effect of (i) the type of carbonaceous materials, (ii) the mixed oxide/carbon ratio and (iii) the nature of active M-Pt assemblies in mixed oxide-carbon composite supports on the electrocatalytic performance of related Pt catalysts. Integration of novel catalysts into membrane electrode assemblies (MEAs) and building of PEM fuel cells and stacks from these MEAs for performance tests under laboratory conditions and for application in new hydrogen powered electronic devices will be demonstrated in the lecture.

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Plenary Pl-14

Plasmon-enhanced fluorescence of emitters: from organic molecules to upconversion nanoparticles.

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Abstract. Plasmonic nanostructures that can direct and amplify light emission of nanoscale emitters provide suitable platforms for linear and nonlinear optics with ultracompact dimensions. The precise positioning, at the nanometer level, of gold nanotriangles and fluorescent dyes, thanks to a DNA origami structure, allowed us to evidence a spectral dependence of the plasmon-enhanced fluorescence in the nanostructure. Based on this structure, we exemplify the operation of a plasmonic router. The collective decay rate of molecular assemblies exhibits spatial modulations in proximity to a metal interface, which we demonstrate both experimentally and theoretically. The generation of anti-Stokes emission through lanthanide-doped upconversion nanoparticles (UCNPs) is of great importance for imaging and labelling applications. However, the weak absorption and long radiative lifetimes of UCNPs may significantly limit their use in such applications. By coupling gap plasmon modes to nanoparticle emitters, we report here the direct observation of upconversion superburst with directional, fast and ultrabright luminescence. Furthermore, by coupling UCNPs with anisotropic gap plasmon mode-supported metasurfaces, we engineered a platform which can switch between four upconversion polarization states, leading to information multiplexing and hence the ability to control the polarization of light essential for information encoding and display technology.

Keynote K-1

Advanced 2D materials: an innovation arena for nanoelectronics, molecular sensing, optical properties, cationic pollutant removal from aqueous solutions

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Abstract. Silicene nanostrips garnered attention due to their physical properties, making them an ideal candidate for electronics and plasmonics applications. Our study serves as a fundamental starting point and a source of inspiration for future experiments, providing a foundation for confirming the results presented here. We then analyse the electronic and plasmonic behavior of periodic planar distributions of sufficiently wide graphene nanoribbons, for which a thorough ab initio investigation is practically unfeasible. Our approach is based on a semi-analytical model whose only free parameter is the charge carrier velocity, which we estimate by density-functional theory calculations on graphene. By this approach, we show that plasmon resonance energies of the scrutinized systems fall in the lower THz band, relevant for optoelectronic and photonic applications. We observe that energies critically depend on the charge carrier concentration, ribbon width, electron relaxation rate, and in-plane transferred momentum angle, thus suggesting a tunability of the associated light-matter modes. Then, an effective model is derived from the ab-initio framework, which reasonably accounts for the two-plasmon response of the studied, ultranarrow nanoribbon systems, at small momentum transfers. The procedure may be extended to more complex nanoribbon heterostructures, thus emphasizing the need for an ab-initio guide to reliable design of nanoplasmonic devices. Lastly, we review the recent results of our group on the effective and efficient removal of cationic pollutants from aqueous solutions using eco-friendly prepared oxidized graphene. This adsorbent material has the advantage of a fast adsorption and keeps a good efficiency over a wide range of initial cationic pollutant concentrations and a broad range of pH values. Thus, we can propose the use of this adsorbent material, as a green adsorbent for wastewater decontamination.

Keynote K-2

Common-path photothermal interferometer for measuring low absorbance

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Abstract. We report a compact photothermal lateral shearing digital holographic device. It is based on the thermal lens effect and a common-path, self-referencing digital holographic microscope comprising a glass plate, probe beam, and a CMOS camera for measuring very low concentrations. The change of phase distribution caused by the temperature change due to light absorption is measured from recorded holograms to extract the sample's absorbance and absorption coefficient. The feasibility of the proposed configuration is validated by the experimental results obtained with different concentrations of gold nanoparticles (AuNPs) in an aqueous solution. Determination of AuNPs concentration at nM range is performed, and the obtained limits of detection and quantitation are 0.04 nM and 0.13, respectively. In addition, the method's versatility is demonstrated by measuring the absorption coefficient of low-loss solvents such as ethanol and water. The determined absorption coefficients agree with the reported values, confirming that this method provides good spectrometric capabilities such as high sensitivity and accuracy.

Keynote K-3

Bioinpired Nanopore Sensors Using Antibody Mimetic Technologies

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Abstract. In this talk, I will dwell on recent developments in nanopore technologies that impact molecular biomedical diagnostics. Significant progress has been accomplished in protein analytics using nanopore-based techniques. However, creating generalizable nanopore sensors to detect proteins at a single-molecule level without the confinement of the pore interior remains challenging.[1, 2] We addresses this long-standing technological difficulty by formulating, developing, and validating a new class of sensing elements in single-molecule protein detection. The key ingredient of this technology is fusing an external programmable antibody-mimetic binder with a monomeric protein nanopore.[3] This strategy drastically expands the spectrum of applications of nanopore sensors to a broad range of proteins and biomarkers without altering their modular architecture, high specificity, and sensitivity. Notably, these nanopores operate in biofluids at clinically relevant concentration ranges of protein biomarkers and with an extended time bandwidth. In this case, the reporting signal unambiguously distinguishes protein recognition events at single-molecule precision without the requirement of utilizing complex analysis algorithms.

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SECTION T1

Stable Isotopes and Emerging Approaches

Oral T1-1

HBCD degradation by sulfidized microscale Fe^0 and its determination by UHPLC-Q-Orbitrap HRMS coupled with isotope dilution analysis

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Abstract. Hexabromocyclododecane (HBCD) is a persistent organic pollutant, well-known as toxic brominated flame retardant, which have attracted wide attention due to its toxicity and increasing level detected in various environmental matrices. This study aims to investigated the degradation of HBCD isomers (α-, β-, and γ-HBCD) by sulfidized iron, by using different sodium sulfide concentrations (0, 1, 5 and 10 mM) and the same amount of 0.6 g microparticle of Fe. The experiment was performed in five anaerobic bottles screwed gas-tight for 14 days, incubated at 30 °C and 125 rpm. For sampling, 10 mL aliquots of HBCD solution were taken at regular intervals, treated with 0.5 mL 37% HCl and 50 µL solution containing ^{13}C-labelled α-HBCD (internal standard) in concentration of 100 ng/mL and then extracted with 3 mL dichloromethane. The organic extracts were evaporated to dryness under N_2. The resulting organic residues were re-dissolved in 1 mL of acetonitrile, then filtered through a 0.45 µm PTFE filter membrane into 2 mL vials for injection in UHPLC-MS-MS system. The analytes separation was carried out on a Kinetex C18 column (100 × 2.1 mm, 1.7 µm), at 30 °C, under the action of a gradient of two mobile phases: A - HPLC water with 0.1% acetic acid and B - methanol:acetonitrile = 70:30 with 0.1% acetic acid, at a flow rate of 0.25 mL/min. The concentration of γ-HBCD in the absence of sodium sulfide decreased from 458.8 ng/L at the beginning of the experiment to 19.9 ng/L after 14 days, while in the bottle amended with 10 mM Na_2S, the γ-HBCD concentration decreased from 861.2 ng/L to 8.6 ng/L, indicating an influence of the hydrosulfide ion (SH^-) on the dehalogenation rate. Various dehalogenation reaction mechanisms must be further investigated.

Acknowledgments. The work has been conducted under the project 584 PED/2022-"New eco-nano-technologies for the elimination of halogenated organic compounds from wastewater using advanced oxidation and reduction processes and anaerobic biodegradation processes", funded by UEFISCDI, Romania.

Oral T1-2

ATR-FTIR and FT-Raman spectroscopy associated with chemometrics for honey authenticity control

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Abstract. Vibrational spectroscopy has been extensively used as a reliable analytical tool in forensics, for the falsification or adulteration detection in food commodities. This is because, FT-IR and FT-Raman spectroscopies are easy-to-use, practical methods with a fast response, that, when paired with supervised statistical tools or artificial intelligence, can generate successful classification models capable to detect the subtle particularities in food or beverages. Honey is one of the most falsified food commodities in the world, and with pollution and environmental issues, many geographical areas have a risk of bee extinction, meaning a diminished production of honey. Moreover, honey loses its aroma and flavour over time. Therefore, it is important to identify pure honey and develop analytical approaches that permit the verification of the quality specification. In this regard, the ATR-IR and Raman spectra of 106 authentic Romanian honey samples gathered during the 2020 and 2021 harvesting years, having four floral sources, were collected. A comparison of the best classification models, capable to differentiate among the botanical origins and harvesting years was conducted, in order to determine which vibrational spectroscopy technique associated with a supervised chemometric tool (partial least squares discriminant analysis, PLS-DA) is more suitable for honey authentication.

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Oral T1-3

Applications of Artificial Intelligence in recognizing the origin of wine based on ^{1}H-NMR spectroscopy

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Abstract. The potential given by the application of Artificial Intelligence in association with ^{1}H-NMR spectroscopy for wine authentication control has been investigated in the frame of the present study. In this regard, two Machine Learning algorithms, namely Support Vector Machines (SVM) and K-Nearest Neighbors (KNN) have been utilized as supervised learning techniques for the development of classification models able to recognize the variety, geographical origin, and vintage of wine. In this regard, a data set consisting of 50 Romanian white wine samples from four varieties (i.e. Sauvignon Blanc, Chardonnay, Pinot Gris, and Riesling) and produced between 2012 and 2016 was employed. Due to the complexity of the experimental data, which was characterized by a large number of variables (i.e. more than 32000 spectral points), special attention was given to the pre-processing phase to identify the most suitable input space for constructing the wine classifiers. A particularly effective approach in this context involved identifying the relevant ^{1}H-NMR variables for each differentiation criterion before model development. The obtained results illustrated that SVM represents a more reliable learning technique for the development of wine classification models as opposed to KNN, leading, in all of the cases, to accuracy scores greater than 94% during cross-validation.

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Poster T1-1

Recent progresses in separation techniques for lithium isotopes – an overview of chemical exchange methods in two liquid phases using crown ethers

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Abstract. In terms of isotopic technologies, it is essential to produce materials with an enriched isotopic abundance, which is one that differs from natural abundance. The separation factor of 6Li/7Li with chemical extraction methods in two liquid phases using crown ethers is comparable to that of COLEX method, due to crown ethers unique cavity structures and size effects. The principle of this separation is that the solvation environment of the cations is quite different when a metal salt is distributed between an immiscible solvent containing a macrocyclic compound and an aqueous solution. Nevertheless, the relatively weak interaction of crown ethers with Li+ leads to a low distribution coefficient of Li (DLi, 10–2–10–5), particularly for crown ethers with small cavities such as 12-crown-4 (12C4), or B12C4. Furthermore, it was demonstrated that due to the dipole–ion interactions between the donor O atoms and Li+, the cavity sizes of free 12C4, 15C5, and 18-Crown-6 (18C6) crown ethers decrease upon their coordination with Li+ ion. Therefore, crown ethers with large cavities such 15C5, 18C6, and DC18C6 could be chosen for their higher distribution coefficient. A more recent strategy (called ion–pair strategy) was developed to create an efficient phase transfer of Li+ by crown ethers. In this system, FeCl3 salt, known as a strong Lewis acid, was introduced for Cl– binding to form [FeCl4]– anion, and B12C4 or B15C5 acted as Li+ receptor. Considering all the above-mentioned facts, this work will try to emphasize the current trends in 6Li/7Li separation by chemical exchange methods in two liquid phases using crown ethers.

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Poster T1-2

Bottled water for babies versus bottled spring water - elemental and isotopic profile

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Abstract. The consumption of essential minerals in adequate quantities is significant for the healthy growth of infants. Bottled water affects the total trace element and mineral intake of infants and toddlers, its content should be known. The lack or excess of elements/minerals?, such as Na, K, Mg, K, Zn, Se, Mn, Fe, Cr or Mo may affect human health. Furthermore, even if the potentially toxic elements (Pb, Cd, As, Hg, etc) reach the body at trace levels, they can accumulate and could lead to negative health effects. In this preliminary study, essential and non-essential element concentrations of bottled water intended for baby's consumption and bottled spring water sold in the local market in Romania were examined. In addition, the hydrogen (δ^2H) and oxygen ($\delta^{18}O$) isotopic compositions of all investigated samples were analysed and evaluated in the context of their origin authentication. Different sources of bottled water in the context of the place of its origin are directly connected with the water quality, marketed brands, and their authenticity. It is possible to differentiate and authenticate bottled waters which have specific isotopic compositions resulting from unique origins connected with geological factors (like water-rock interaction or admixture of water of non-meteoric origin).

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Poster T1-3

Biochar – a green and versatile carbon-rich material

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Abstract. Sustainability is the ability to exist and develop without depleting natural resources for the future. Biochar is a low-cost porous material rich in carbon derived from the thermochemical degradation of biomass. This work aims to study this material obtained by pyrolysis over 550°C from eggshells, Pelargonium leaf, orange peel, coffee zest, pistachio shells, apple tree branches, and snail shells. The samples obtained were analyzed and morpho-structurally characterized using the BET method and X-ray diffraction. Optimization of biochar synthesis for improved properties (specific surface area and pore size) make this material have great potential as a green catalyst in different chemical syntheses, as an effective, ecologically friendly adsorbent for organic and inorganic contaminants, and as an electrode modifier for electrochemical detection of analyte from medicine, agriculture, and environment.

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Poster T1-4

New random packing modular testing plant for ^{18}O isotope separation through H_2O vacuum distillation

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Abstract. A new ^{18}O isotope modular separation plant, adjusted for different experiments was designed and it's purpose is to test different types of random packing with different shapes and materials. A proper monitoring and control system was developed to allow the column to work with any number of modules; each module being approximately 1m high and equipped with temperature and pressure sensors, water inlet and outlet valves and sample port. At the bottom, evaporation of water is precisely controlled and at the top, a condenser recirculates the water down for a complete cycle. With this new modular testing plant the separation performances of random packings will be determined.

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Poster T1-5

Fatty acids profile and metals content in selected sorts of cookies and biscuits, offered children's

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Abstract. Cookies and biscuits are very popular ready-to-eat foods due to their affordable cost and long shelf life. These processed foods may contain a complex mixture of fats from sources such as vegetable oils or/and animal fats, besides hydrogenated or partially hydrogenated oils. In recent years, particular attention has been paid to the adverse effects on human health from the consumption of foods containing saturated fatty acids (SFAs) and trans fatty acids (TFAs). TFAs increase the risk of cardiovascular diseases, by increasing LDL-cholesterol and decreasing HDL-cholesterol, which leads to the displacement of essential fatty acids from membranes. The food products elaborated with hydrogenated fats, such as margarine, cookies, and other industrially baked products, are highlighted as the main source of TFA in the diet. Besides this, these food items may contain heavy metals picked up from the ingredients, production methods, or packaging. Foods for children must not contain contaminants at levels that could cause adverse health effects. Considering this, the present study presents the obtained results in regard to the composition of fatty acids and metals in some brands of cookies and biscuits commercialized on the Romanian market. The composition in fatty acids (FA), with emphasis on the content of TFA, was determined by gas chromatography with a detector with flame ionization (GC-FID). Inductively Coupled Plasma Mass Spectrometry (ICP-MS) analysis was used to determine the concentration of metals.

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Poster T1-6

Stables isotopes and elemental fingerprints are enough to identify the geographical origin of pork?

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Abstract. Pork is one of the most commonly consumed meats in the world. In Romania, there is a strong tradition both for breeding pigs and pork consumption. The consumption rate reached 37.3 kg per capita in 2020. In the context of African swine fever and price increases, consumers pay more attention to the meat they eat, especially related to its geographical origin that is usually associated with either a quality given by the lack of pollution in that region, or to a different growth regime, such as food without feed concentrates/ pasture breeding. In this study, the isotopic ($\delta^{2}H$, $\delta^{18}O$, and $\delta^{13}C$) and elemental signatures (macro-, microelements, metals with toxic potential) of 100 samples of pork meat were recorded. By applying a statistical treatment to the entire data set, classification models were developed and differentiation markers were obtained for assigning the geographical origin of meat and animal breeding system (animals coming from yard rearing system versus animals coming from industrial farms).

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Poster T1-7

Quality and safety assessment of commercial infants and toddlers foods

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Abstract. Because the first year of a child's life represents a very vulnerable and sensitive period in human development, it is necessary that the food products intended for this age category ensure high quality and safety standards. In the last period, the number of infants and toddlers who are fed commercially available purees from fruit and vegetable or meat products has increased more and more. In this context, the present study aimed to evaluate: 1) the elemental profile (minerals and potentially toxic elements); 2) the isotopic content ($^{13}C/^{12}C$); 3) the lipid profile, and 4) the aroma compounds of different commercial baby food. The methodology comprised the inductively coupled plasma mass spectrometry (ICP-MS) analysis for elemental concentration; isotope ratio mass spectrometry (IRMS) for the isotopic fingerprint of ^{13}C; gas chromatography with flame ionization detection (GC-FID) for lipid profile and headspace solid phase microextraction (HS-SPME) coupled to gas chromatography mass spectrometry (GC-MS) in identifying of volatile compounds. Furthermore, the aim of this pilot study was to assess potential health risks (non carcinogenic) for infants and children less than 1 year resulting from consumption of investigated products. The estimated daily intake (EDI), target hazard quotient (THQ), and hazard index (HI) were evaluated.

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Poster T1-8

Quantification of pesticide residues in frozen fruits and vegetables by GC-ECD and HPLC

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Abstract. Quantification of pesticide residues in frozen fruits and vegetables is a crucial process to ensure the safety and quality of these food products. Pesticides are chemicals used to control pests and diseases in agricultural practices, but their presence in food at high levels can pose health risks to consumers. Gas Chromatography with Electron Capture Detection (GC-ECD) and High-Performance Liquid Chromatography (HPLC) coupled with various detection systems including ultraviolet and mass spectrometry (MS) are two commonly used analytical techniques for pesticide residue analysis. GC-ECD is a powerful analytical method that separates and detects volatile and semi-volatile organic compounds. In the context of pesticide analysis, the frozen fruit or vegetable sample is first extracted to isolate the pesticide residues. When combined with the QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) sample preparation method, they provide effective and reliable results. Therefore, the aim of our study was to develop an accurate, sensitive, and economic QuEChERS combination with HPLC and GC-ECD methods for the quantification of pesticide residues in frozen fruits and vegetables. The obtained sensitivity, linearity, recovery, and LODs have been estimated and then evaluated with respect to the current requirements of the EU. The limit of quantification for the selected pesticides was lower than the maximum residue limits (MRLs) set by European Union, Codex Alimentarius Commission (CAC), and other countries. By comparing the obtained results with MRLs, it can be determined if the samples comply with pesticide regulations and are safe for consumption.

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Poster T1-9

Ruthenium type catalyst for selective deuteration of amino acids

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Abstract. In order to develop synthetic methods for easy access to deuterated materials, an α-selective deuteration of amino acids has been approached using ruthenium on alumina catalyst, deuterium oxide as a source of deuterium in hydrogen gas atmosphere. For the specific deuterated amino acids, good yields were obtained and also highly deuterium incorporation was proven. Selective deuterated amino acids can be used in medical imaging, in the development of new drugs or in investigations of reaction mechanisms in organic chemistry or biochemistry.

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Poster T1-10

Data fusion – a new approach for food differentiation

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Abstract. Honey is one of the most counterfeited commodities, particularly certain types, as there are limited accessible amounts and high market demand. This is due to the fact that some of the most essential characteristics of honey, whether in terms of flavor or medicinal benefits, are closely tied to its botanical and geographical origin. As a result, the temptation for certain unethical producers or dealers to market honey under fraudulent declarations of botanical variety or geographical origin must be prevented through the development of simple and dependable techniques for honey authenticity management. Vibrational spectroscopy (IR and Raman) in combination with improved statistical approaches has shown to be a good contender for this purpose in recent years.

This study discusses the construction of honey authentication models through the application of data fusion techniques, namely by using the correlation between IR and Raman spectra for defining the input data. Furthermore, the study emphasizes the significance of the preprocessing phase in improving the performance of the constructed models. Aside from that, in order to improve the classification accuracy of the honey discrimination models, a supervised feature selection step was performed to identify the most relevant markers that allowed the samples to be classified according to some pre-established criteria.

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Poster T1-11

Isotopic and elemental fingerprint – an effective association for vegetable authentication

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Abstract. Vegetables are an important part of a healthy eating pattern and are excellent sources of many nutrients. Romania is recognized for its high potential for growing field vegetables, with vast soil fertility and a diversity of weather conditions. Consumption of vegetables in Romania is expected to increase slightly in the next five years, with an average growth of 0.3% year-on-year. In 2021, our country recorded a production of 4 million tons of vegetables. But, also, Romania is a great importer of fresh vegetables from countries like Turkey, Greece, Spain, Italy, Poland, and the Netherlands. Many consumers prefer autochthonous vegetables, for their stronger taste and aroma. In this context, by using Isotope Ratio Mass Spectrometry (IRMS) together with Inductively Coupled Plasma-Mass Spectrometry (ICP-MS), the isotopic and elemental profiles of different vegetables (potato, carrot, lettuce, cucumber) were determined. The aim of the study consisted in the identification of legumes geographical origin and the differentiation of vegetables that grow above ground (lettuce, cucumber) versus those that grow underground (potato, carrot).

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Poster T1-12

Determination of emerging contaminants in drinking water sources

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Abstract. The drinking water contaminants comprise a vast number of natural and anthropogenic substances introduced only recently in the environment or present for a long time. These compounds include industrial and household chemicals, pesticides, manufactured nonmaterial and their transformation products. Very recently, the EU Council approved the proposal to revise the Drinking Water Directive, which updates quality standards and introduces the watch list which including for the first time endocrine disruptors and pharmaceuticals (EU Council, 2020). Organic compounds occurrence in drinking water is a challenge to the environment and human health. The purpose of this study was to evaluate the occurrence of selected chemical compounds in sample collected from sources of drinking water, including also sample of top water. The study is focused on compounds from following families: pesticides, polyflouroalkyl substances (PFAS), polyaromatic hydrocarbons (PAHs), alkyl phenols (APs), pharmaceutics and hormones. The compound analyses were carried out by GC/MS system.

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Poster T1-13

SERS discrimination of small berry fruits varieties

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Abstract. The goal of the present work was to effectively distinguish between various types of small berry fruits acquired from Romanian markets based on Surface-Enhanced Raman Spectroscopy (SERS) spectral data in conjunction with a supervised statistical method, namely Partial Least Squares-Discriminant Analysis (PLS-DA). This approach yielded dependable differentiations among the samples, enabling us to identify the main compounds of the fruit varieties. To identify the primary spectral ranges responsible for differentiation, the samples were categorized into four groups based on their botanical origin (strawberry, raspberry, blackberry, blueberry). The entire Raman spectral range of all samples was employed as input data. Remarkably, an accurate classification of 97% of the samples was achieved using this data, with only one blackberry sample wrongly attributed to the raspberry group. Among the entire spectral range, 366 markers emerged as highly effective indicators for this differentiation purpose.

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Poster T1-14

The study of changes in the composition of stable isotopes of eggs at different storage temperatures.

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Abstract. Stable isotopes have become an accepted method to track resource acquisition and nutrient utilization by birds. The popularity of chicken eggs is increasing worldwide, increased production is expected over the next few years, and it appears that protein production from eggs is more sustainable than other protein rich food production, such as beef. Hence, systems/tools are needed to ensure and guarantee egg traceability along the full chain to provide safe and high-quality food for the consumer. The aim of this study was to assess the potential of the $\delta^{18}O$ and $\delta^{2}H$ values changes as traceability markers for egg storage. Thus, the isotopic fingerprints of ^{2}H and ^{18}O from the extracted water from 60 chicken eggs, summing 120 samples (60 egg white and 60 yolks) were determined by a Liquid Water Analyzer. From each batch of eggs, one sample was prepared and analyzed on the day of the sample's arrival in the laboratory, and its pair after 28 days of storage. The storage temperature was 20°C for a part of the egg samples, and the rest was stored at 5°C. The isotopic composition recorded different values as function of storage temperature.

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Poster T1-15

Methods for characterization of random packings used in isotope separation

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Abstract. Several methods for characterization of the packings used in the separation columns are presented in the specialized literature. In this work, we describe the adaptation of these methods to characterize the random packings used in isotopic separation. We have optimized methods for routine determinations of the structural and operational characteristics of triangular spiral rings, such as packing density, void fraction, specific surface area, loading factor, static liquid holdup and pressure drop. To evaluate the wettability of the studied random packings a contact angle determination method was developed. Several random packings were characterized.

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Poster T1-16

Optimum design of multi-stage separation cascades for oxygen isotope separation

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Abstract. A process for the separation of oxygen stable isotopes, ^{16}O, ^{17}O and ^{18}O, by vacuum rectification of H_2O, using the general theory of isotope separation in cascades was studied. To achieve the optimum design of a real separation cascade, the so-called square cascade, in the first step the external and internal parameters for an ideal cascade were determined. Since in industrial technology it is not possible to achieve ideal cascade conditions, in the next step square cascades from countercurrent separation columns were designed and the cascading yield was maximized.

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Poster T1-17

Elemental content and stable isotope fingerprinting of potatoes from Romanian market

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Abstract. Analytical techniques represent important tools for the quality control in the food security field, where robust, fast and accurate methods are required. Among other pathways, food represents one of the main sources of consumer exposure to heavy metals. Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) based multi-elemental profiling was performed to assess the quantitative complement of toxic metals and essential mineral elements (Zn, Cu, Mn, Ni, Fe, Cr, Pb, Cd) for 60 potatoes. Samples were collected both from the cultivation fields of farmers from various locations of legumes growing in Romania, and from supermarkets (foreign origin). Alongside with elemental content, the isotopic signature of ^{2}H, ^{18}O, and ^{13}C was determined by Isotope Ratio Mass Spectrometry (IRMS). Then, chemometric treatment was applied for the entire data set, in order to differentiate the geographical origin of potato samples and to identify the best markers which emphasize Romanian potatoes.

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SECTION T2

Molecules, Biomolecules and Photonics

Oral T2-1

Polydopamine photochemical behavior under UV irradiation

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Abstract. The UV absorption spectra of polydopamine (PDA) has been experimentally investigated considering different solvent environment and pH conditions. In the second step, first-principles quantum theory was applied to find the most appropriate theoretical method to describe the excitation spectra and the geometries of the ground and excited states of PDA. Accordingly, the ωB97X-D3BJ exchange-correlation DFT functional was found to be the most suitable method, able to describe both molecular geometries and excitation spectra consistently well. Using this theoretical framework, several structural isomers of PDA consisting in protonated and deprotonated fragments inside the PDA chain have been identified and based on these results, a detailed analysis of the different absorption spectra obtained under different experimental conditions has been given. The correlation between the theoretical results and the experimental data allows us to explain the photochemical behavior for different protonated polymer forms.

Oral T2-2

Advances in electrochemically-assisted SERS sensing

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Abstract. Discovering surface enhanced Raman scattering (SERS) from an electrochemically (EC)-assisted experiment was regarded a significant milestone. Raman spectroelectrochemistry (SEC) has evolved into a widely used technique for investigating the electrode/electrolyte interface. In recent years, notable advancements have been achieved also in the field of quantitative analysis, positioning Raman SEC a promising alternative for conventional analytical methods in trace analysis. EC coupled with SERS offer numerous advantages. Tuning the potential of the EC-SERS substrate can effectively modulate both the electromagnetic and chemical effects, leading to significant Raman signal amplification. Moreover, affinity-based or electrophoretically-driven adsorption of analytes or desorption of interferents could improve detection selectivity. As such, EC could enable analyte preconcentration, improve reproducibility or even allow reusability. Additionally, EC techniques may serve as a tool for fast generation of SERS substrates by surface roughening/activation of mass-produced and cost-effective, screen-printed electrodes, representing a convenient and ready-to-use alternative to commercially available SERS substrates. In this work, some guidelines in the activation and selection of EC-SERS substrates are discussed along with particularities and challenges of EC-SERS multiplexing with special attention given to pesticides and pharmaceutical pollutants. Furthermore, the opportunities offered by the packaging of SERS substrate/electrode into microfluidic platforms will also be briefly outlined.

Oral T2-3

Expression, purification and characterization of FlgL protein from *Campylobacter jejuni*

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Abstract. Flagellar hook-associated protein FlgL is a key component of bacterial flagellum ensuring the flexible connection between the filament and the hook. At *Campylobacter* in addition to conferring mobility the flagellum has the role of exporting proteins with significant role in virulence. Consequently, biochemical and structural insights on the corresponding flagellar components are important for exploring alternative ways of fighting *Campylobacter* infections. Recombinant FlgL from *Campylobacter jejuni* was expressed, purified and characterized. FlgL characterization was performed by electrophoresis, size exclusion chromatography combined with multi-angle light scattering, circular dichroism spectroscopy and screening of crystallization conditions. The optimal conditions to produce monomeric and stable FlgL were found and the assessment of protein crystallization parameters was carried out. My research represents a starting point for further structural studies.

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Oral T2-4

The perspectives of numerical neuroevolution of artificial neural networks with applications to Fourier and Laplace-like spectroscopy

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Abstract. Nowadays, the impact of artificial intelligence on many life aspects (from supermarket to science) is more and more noticeable. In particular, the artificial neural network (ANN) is defined as a numeric machine able to be trained to learn by examples and can perform from simplest to complex tasks. Such a trained ANN becomes capable to process rapidly large amounts of data in order to solve problems and can provide educated prediction in real time. An ANN can be successfully used for types of problems where it is difficult to provide a simple-model solution. While ANNs are commonly implemented for image, speech or posture recognition, we will discuss the use of an ANN to analyse spectroscopic data. The general architecture of an ANN and the simplest implementation into a program written in JavaScript using the machine learning library, ml5, are briefly discussed. The limitation in the training of an ANN, in particular due to the random initialization of elements of specific matrices bounding various layers of ANN are highlighted. The solution presented as the implementation of neuroevolution of ANN is discussed. This imply that instead of creating a singular ANN which is tried to be trained, using many examples and taking a long time, many times unsuccessfully, neuroevolution assumes the creation of a population, for which, each element (in this case an ANN considered as DNA) is trained for a short period of time and the result is evaluated. The elements of weights/matrices of ANN are the genes which are passed to the next generation of ANNs with a probability proportional to a fitness score. In order to ensure a sufficient variation the genes' crossover and mutations procedures are implemented. The application of neuroevolution for i) the ill conditioned problem of inverse Laplace transformation which is intensively used in the analysis of multi-exponential NMR data and ii) deconvolution of Fourier spectra (NMR, FT-IR or XRD) are discussed.

Poster T2-1

Long-range order and photonic effects in colloidal microsphere arrays obtained by convective self-assembly *vs* air-water interface self-assembly

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Abstract. Colloidal crystals, i.e. ordered 2D or 3D arrays of colloidal microspheres, posses intriguing, fundamentally relevant optical properties. At the same time, they are highly useful as templates or lithographic masks for the fabrication of various nanostructured metallic patterns. This study presents a comparison between two of the major methods for colloidal self-assembly, namely convective self-assembly (CSA) and air-water interface self-assembly (ISA). Aiming to obtain large-area uniform 2D colloidal arrays with a narrow-band photonic response in the visible spectral domain, advantages and disadvantages of the two methods are analyzed. Thus, colloidal films are prepared by both methods, from colloidal suspensions of polystyrene spheres with a diameter of 460 nm. By collecting both microscopic and macroscopic transmission spectra, the optical response of the self-assembled colloidal photonic crystals was determined, and correlated with morphological analyses and FDTD electromagnetic simulations.

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Poster T2-2

Antimicrobial peptides interaction with model and mammalian membranes

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Abstract. Antimicrobial peptides (AMPs) are one of the novel atimcrobial agents witht promising results against a brod spectrum of *Gram negative* and *Gram positive* bacteria, even multiresistant bacteria. However one of their main drowbacks, for some of the AMPs, is increased toxicity towords mammalian cells. A better understanding of the complex mechanism related to the interactions between the AMPs and mammalian membranes can become an important parameter which could help to develop more suitated peptide for clinical therapy.

In this study we used biophysical techniques to investigate the interation between AMPs and model as well as mammalian membranes. Membrane fluidity was investigate using Laurdan steady-state fluoresnce. Several parameters were used to characterize the membranes when the peptide was added: generalized polarization (GP), the difference between the relative areas of elementary peak (ΔSr), and the ratio of elementary peaks areas (Rs). The parameters can destinguish the changes generated by peptide addition as well as between different membranes investigate.

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Poster T2-3

Modulation of gold nanoparticle morphology for improved loading of therapeutic oligomers

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Abstract. Oligonucleotide-based drug platforms are currently being explored for their potential therapeutic applications in various diseases including neurodegenerative disorders and cancer. A major translational limitation is to achieve the efficient delivery of oligonucleotides, particularly to extrahepatic tissues and to retain their functionality for modulating gene expression. To address the delivery challenge, we explore the use of nanocarriers, herein gold nanoparticles, and modulate their physico-chemical characteristics such as size, shape and surface chemistry. For a better understanding of the intramolecular mechanisms involved in particle functionalization, the nanoparticle-oligonucleotide conjugates were studied through molecular dynamics simulations using both atomistic (AA) and coarse grained (CG) models compatible with the CHARMM and MARTINI force field, respectively. Different surface coverage densities are compared both theoretically and experimentally. The results show that a variation of the oligonucleotide density in the design of functionalized gold nanoparticles leads to differences in the DNA strands packing, and hence influences the loading efficiency of the cargo molecules.

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Poster T2-4

Rapid and reliable chromatographic profiling of thiosulfinates in *Allium* species

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Abstract. Allicin (diallylthiosulfinate) is a highly reactive sulphur containing compound, found in several *Allium* species. Allicin is synthesized on an enzymatic pathway during smashing garlic, starting from S-allyl-l-cysteine sulfoxide (alliin). Allicin determination can be performed using spectrophotometric and HPLC techniques. The aforementioned methods have limitations regarding interferences caused by other thiosulfinates (spectrophotometric method) and the high-cost equipment and highly trained analysts required in the case of HPLC-DAD-MS. The purpose of this work is to present a simple and sensitive analytical method for the simultaneous detection of alliin and allicin, based on SAMC formation followed by digital subtraction thin layer chromatography. Allicin is quickly pre-derivatised with cysteine in excess to the stable S-allylmercaptocysteine that is then simultaneously detected with alliin, using ninhydrin reagent. The method was validated in terms of accuracy, precision, selectivity, robustness, peak purity and limit of detection. In addition, we show here that this method can be extended to other thiosulfinates and thus allowing a profiling of these important analytes in *Allium sp.* Moreover, we show that replacing cysteine with other derivatization agents, thiosulfinates profiling could be improved. The method was successfully applied using real *Allium sp.* samples and the results were in good agreement with HPLC data.

Poster T2-5

Immuno-detection of cancer biomarker CEA-CAM5 using SERS-active gold nanourchins

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Abstract. Anisotropic plasmonic nanoparticles such as gold nanourchins (GNUs) are excellent platforms for Surface-enhanced Raman spectroscopy (SERS) detection due to the high electromagnetic fields concentrated on their multiple spikes, generous surface area and accessible surface chemistry. In this work, we fabricated Raman reporter (Rr)-encoded, anti-CarcinoEmbryonic Antigen-related Cell Adhesion Molecule 5 (CEA-CAM5) antibody conjugated GNUs that can serve for the detection of CEA-CAM5 cancer biomarker with high affinity and specificity. The polyclonal antibody binds the target protein at various sites, allowing different particles to become adjacent through a target protein, resulting in particle-protein-particle sandwich structures, which further modulate the signal enhancement in the created hot-spots areas. The enhancement in SERS signal of the Rr and the target protein concentration are thus correlated, allowing biomarker quantification. Further on, the analyte detection was studied in an "in-flow" microchannel platform, an approach with potential for better portability and miniaturisation.

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Poster T2-6

Fabrication of Highly Sensitive and Selective SERS-active Nanostructured Plasmonic Platforms

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Abstract. A very promising tool for the non-destructive detection of selective analytes at ultra-low concentrations is surface enhanced Raman scattering (SERS) technique. The fingerprint of the detected samples can be obtained with high specificity and sensitivity when using a metallic nanostructured substrate with plasmonic features. In our work, we fabricated high quality SERS detection platforms based on self-assembled films of polystyrene on glass by employing nanosphere lithography (NSL) method. Silver (Ag) films with tunable thicknesses were deposited by molecular beam epitaxy (MBE) technique on room temperature on polystyrene nanospheres with diameters of 607 nm and 800 nm, respectively. The deposition parameters such as deposition time and rate were optimized based on the scanning electron microscopy (SEM) images. Atomic force microscopy (AFM) revealed defect-free, homogeneous and uniform metallic films, with low roughness.

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Poster T2-7

Experimental and numeric simulation used for the characterization of nanofibers biomaterials produced by electrospinning

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Abstract. Nowadays electrospinning is an increasingly used technique for producing nanofibers from various types of polymers and biopolymers. These fibers become suitable for modern applications in tissue engineering, wound healing and drug delivery. In this study, we focused on four different biomaterials produced from raw marine collagen, chitosan and polyvinyl alcohol (PVA). Various collagen/chitosan, PVA/chitosan and collagen/chitosan/PVA in different ratios were dissolved in acetic acid. The formed solutions have the concentrations in the range from 2 - 90 % (g/ml). The effect of different molecular format (e.g. native and denatured collagen) was studied. The prepared solutions were used in electrospinning experiments. The bio-polymeric solutions were placed into a 50 ml syringe with a needle of 0.8 mm inner diameter. The high voltage power supplier (12 kV) was connected to the needle via a conductive clamp. The feed rates of the solution were optimized. The raw materials, bio-polymeric solutions and finite nanofibers biomaterials were characterized using several techniques, such as: FT-IR spectroscopy, scanning electron microscopy (SEM), low-field NMR relaxometry and high field ^{1}H, as well as NMR imaging and single voxel ^{1}H NMR spectroscopy. The degree of crystallinity was established from X-ray diffraction measurements. To analyse the SEM images, we employed artificial neural network (ANN), based on machine learning library (ml5). In this sense the ANN was trained to identify structures and patterns. The overall study was proved to be helpful for a better understanding of the produced nanofibers properties. This study demonstrates the potential of electrospinning for producing nanofibers and highlights the importance of using multiple characterization methods for a better understanding of the bio-fibers properties.

Poster T2-8

SERS-based monitoring of the efficiency of new generation antimicrobial agents

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Abstract. Raman and in particular surface-enhanced Raman scattering (SERS) techniques have developed into emerging biomedical tools with a real aid to differentiate and discriminate subtle spectral differences of antibiotic-resistant and susceptible bacteria. The SERS sensitivity down to single bacteria detection, the portability and ease-to-operate makes it appealable for real life applications. Among the changes that can appear in the Raman/SERS spectra of sensitive, susceptible or resistant bacteria are the cell wall structure variations determined by the antimicrobial peptide action. Our work focused on the application of Raman spectroscopy to identify the fingerprint of *E. coli* deposited on mica substrates. Furthermore, *E. coli* samples were treated with antimicrobial peptide P6 and the possibility for Raman detection of the susceptible bacterial mass was assessed. The preliminary results were compared with the bacterial single-cell SERS profiles obtained by using conventional antimicrobial agents, such as 5th generation beta-lactamic antibiotics.

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Poster T2-9

Intermolecular interactions in uric acid cluster

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Abstract. The formation of uric acid crystals has received little attention from the scientific community. The form in which the uric acid crystallizes is called lactam and from all forms of tautomers, the lactam form has the most stable form. In this way, the structural stability and the charge transfer effects were investigated using DFT and MP2(DLPNO-SCS-MP2) methods. For the DFT method the functional wB97X-D3 together with the def2-TZVP basis set were chosen, while for the MP2 theory the DLPNO-SCS-MP2 method provide accurate results for our systems. The stacking-type dimers and the cyclic-hydrogen bonds have been identified. Also, the nature of the intermolecular interaction energy has been studied. In the case of experimentally obtained crystalline structures[a], the nature of the intermolecular interaction energy has been investigated between the crystalline units.

Poster T2-10

Computational design optimization of gene delivery vectors for the CRISPR/Cas9 systems

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Abstract. CRISPR/Cas9 therapy, which has a variety of benefits over traditional gene therapies, can be used to effectively modify specific genes. The main challenge in using the CRISPR/Cas9-based approach is creating gene delivery vectors that can target specific mutations in the genome. CRISPR/Cas9 has been delivered in vivo to treat inherited illnesses such muscular dystrophy using gold nanoparticles functionalized with oligonucleotides. Because current CRISPR/Cas9-Gold treatment trials are in the early stages of development, delivery vectors with minimal insertional mutagenesis risk should be created based on molecular knowledge of the implicated systems. First, in nanoparticle-oligonucleotide conjugates, we optimized the DNA loading on a variety of GNP sizes. In the subsequent stage, we simulated the Cas9-sgRNA complex using molecular dynamics. This study is crucial for improving the gene delivery system based on CRISPR/Cas9-Gold.

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Poster T2-11

Mechanically tunable, polarization-dependent plasmon resonances in linear oligomers of gold nanospheres

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Abstract. Controlling surface plasmon resonances of metal nanostructures if of great importance for developing several high-sensitivity optical sensing applications. Moreover, active tuning of these resonances allows to control in real-time the spectrum of the near-field enhanced electromagnetic fields, and thus to control the optical interactions between molecules and the metal surface. In this work, we explore by Finite-Difference Time-Domain electromagnetic simulations the plasmonic response of linear oligomers made of gold nanospheres. The optical response of linear arrangements such as dimers, trimers, and quadrumers is obtained for different sphere sizes, interparticle gaps, and polarization of the incident light. In view of plasmon-enhanced optical spectroscopy applications (e.g. surface enhanced Raman/fluorescence), the sensitivity of both dipolar and quadrupolar coupled plasmon modes to interparticle gap variation is evaluated. The achievement of both red-shifting and blue-shifting plasmon modes offers way to mechanically alter the optical response of the linear oligomers in real-time, and design new optical sensing approaches.

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Poster T2-12

In-silico analysis of potential inhibitors of eye lens γ-crystallin aggregation and cataract prevention

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Abstract. Cataract, the leading reason of blindness worldwide, is characterized by the presence of a cloudy area in the eye lens resulting in a loss of transparency. Cataracts often develop slowly and are most commonly due to aging or can also be present from birth due to congenital mutations. A number of mechanisms contribute to the longevity and transparency of human lens, a reducing and oxygen deficient environment, the presence of UV-filters, and most importantly a unique supramolecular organization of its structural proteins, the α-, β- and γ-crystallins. The high concentration of γ-crystallin proteins of about 400mg/ml is close to spontaneous crystallization that is prevented by the presence of molecular chaperones α-crystallins. With advancing age, progressively, or due to some mutations, this fragile equilibrium can be perturbed, causing γ-crystallin insolubilization, unfolding, fragmentation and aggregation. In this study, we performed a careful comparative *in silico* analysis to find potential molecules of natural origin, which might protect γ-crystallins from destabilization and aggregation. Our specific protein targets are wild-type human γD-crystallin and its mutant P23T γD-crystallin, associated with congenital cataract.

Poster T2-13

Convolutional neural network for randomly shaped ultrashort pulse characterization

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Abstract. Ultrafast laser pulses are used in various fields such as high-harmonic spectroscopy, femtochemistry or ultrafast imaging. In these applications the pulse characterization (amplitude and phase) is highly important, SHG-FROG being one of the techniques used. In this case, a spectrogram image is recorded and the amplitude and phase of the ultrashort laser pulse are retrieved by algorithms like PCGPA or ptychographic FROG. A disadvantage of using these techniques is that they can be time consuming and their convergence is not guaranteed. Artificial neural networks are known to be high speed mathematical models. Thus, in this work, we propose laser pulse characterization by using convolutional neural networks (CNN). The neural network data consists of a multitude of FROG traces which originate from randomly shaped pulses. The developed CNN retrieves the laser pulse in just tens of millisecond, whereas the error between the initial retrieved pulses and the CNN predicted pulses has low values.

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Poster T2-14

Molecular Modeling and Simulations Play a Key Role in the Design of Novel Anti-Cancer Peptides

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Abstract. Ras proteins are small GTPases that function as molecular switches between the GTP-bound active and GDP-bound inactive states in the signal transduction pathways which regulate cell proliferation, differentiation and growth. Wildtype Ras oligomerize into dynamic lipid-bound nanoclusters that respond to cellular input signals and local membrane fluctuations. Hence, over 85% of their mutations are oncogenic, and are responsible for ~20% of all cancers. The poor clinical outcome of oncogenic Ras treatments makes finding novel oncogenic Ras inhibitors as top priority in the oncogenic line of research. Here we used *molecular modeling and various theoretical approaches and simulations* as key tools in (i) *understanding* the underlying processes involved in Ras' dynamic *nanoclustering*, and in (ii) *designing of novel peptides that act as oncogenic Ras inhibitors*. Ras association free energy calculations, peptide (ligand) – Ras (receptor) molecular docking calculations, and the most efficient peptides – Ras complexes' molecular dynamics simulations were found to be efficient tools in designing novel anti-cancer peptides.

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Poster T2-15

Investigation of Vitamin C and β-cyclodextrin interactions in liquid and solid state

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Abstract. The inclusion complex between Vitamin C (ascorbic acid) and β-cyclodextrin in both liquid and solid state was pursued for oral extended-release product. Based on the chemical shifts observed by ^{1}H-NMR spectroscopy in aqueous solutions of Vitamin C - β-cyclodextrin mixtures in different molar ratios, the association constant value suggests weak interactions between the components. The results of isothermal calorimetry measurements show a low affinity of vitamin C towards β-cyclodextrin, an observation also supported by molecular docking simulations. The solid state Vitamin C - β-cyclodextrin inclusion compound was prepared using various conditions and methods and characterized using dedicated techniques. It was observed that the inclusion compound obtained in 1:1 molar ratio by freeze-drying was successful, resulting in an amorphous material whose characteristics highlighted by X-ray powder diffraction, FTIR spectroscopy and differential scanning calorimetry, are clearly different from those of the initial substances.

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Poster T2-16

Femtosecond laser pulse filamentation in air

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Abstract. Filamentation is a process which makes possible the long-range propagation of intense laser pulses in air. Due to this property laser pulse filaments find application in defence technology, atmospheric research, meteorology, pollution study. We study the process of filamentation at fundamental level. Using our numerical model for laser pulse propagation which calculates the propagation of the full electric field, we have the opportunity to perform a fundamental investigation of the different competing processes which lead to the creation of laser filaments. Mainly, there are two competing effects: the optical Kerr effect which acts as a converging lens, and the plasma defocusing which acts as a divergent lens. In the case of a dynamic equilibrium between these two, a self-guiding propagation regime can be established. The main advantage of our model is that it gives the opportunity to separately investigate the Kerr effect, the plasma dispersion, neutral dispersion, geometrical focusing, effect of gas pressure, pulse energy, etc. Self-steepening is the temporal shortening of the laser pulse during self-guided propagation. This property is used for pulse compression in laboratories where ultrashort laser pulses are needed. In this work we present our recent results in collaboration with the group of prof. Hyung Taek Kim from APRI, Gwangju, Korea. Experimental evidences of femtosecond laser pulse filamentation are explained using our mathematical model and simulation.

Poster T2-17

Assessment of cymoxanil residues in selected fruits and vegetables using HPLC–PDA/MS

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Abstract. Pesticides are used primarily for pest control that can occur in plants, but besides beneficial effects, their use has a negative impact on the human health and environment. Due this, the quantification of pesticide residues in fruits and vegetables has become a necessity. The purpose of this work was to determine the content of cymoxanil residues in some fruits and vegetables (apples, grapes, oranges, strawberries, tomatoes, cucumbers, onion, spinach, lettuce, potatoes, radishes and cabbage). The cymoxanil was extracted from samples using a solution of acetonitrile with 0.1% ammonia and the complex matrix samples were purified with multi-walled carbon nanotubes. The content of cymoxanil residue extracted from the selected samples was assayed by HPLC-PDA/MS analysis. The chromatographic separation was carried out on a NUCLEODUR C18 HTec column (100 × 3 mm, 3 µm) at 30 °C. The elution of the cymoxanil was achieved with acetonitrile-water containing 0.1% formic acid (60:40, v/v) of mobile phase at a flow rate of 0.3 mL/min. Cymoxanil residue was detected in tomatoes, onion, cabbage and radishes.

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Poster T2-18

Plasmonic nanostructured substrates fabricated by colloidal lithography for nanoplastics SERS detection

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Abstract. Surface-enhanced Raman spectroscopy (SERS) is a well-known analytical technique widely applied for the identification of numerous chemical substances such as drugs, biomolecules, and pollutants. The performance of nanostructured solid SERS substrates is strongly depended on structural arrangement and geometry of surface nano-micro-scale features. In this respect, a class of quasi-3D nanostructured SERS substrates were fabricated by means of colloidal self-assembly, plasma-etching, and e-beam evaporation of noble metal thin films. The developed colloidal lithography technique is relatively simple, low-cost, and highly-efficient in fabricating uniform, large-area plasmonic crystals with optimal features for SERS applications. The plasmonic response of the nanostructured substrates was analyzed by reflectivity measurements and corroborated with electromagnetic FDTD simulations. A detailed characterization of the SERS enhancement was carried out by the Wavelength-scanned Surface-enhanced Raman spectroscopy (WS-SERS) in the NIR-IR spectral range. The SERS capability of the plasmonic substrates was explored in the detection of nanoplastic, a pollutant of great concern today.

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Poster T2-19

Ketoconazole-PAMAM dendrimer carrier system for topical use

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Abstract. Ketoconazole (KTZ) is the first broad-spectrum oral antifungal Active Pharmaceutical Ingredient approved by FDA. Its high lipophilicity and extremely weak basicity contributes to its poor aqueous solubility, insufficient to dissolve the administered dose under normal conditions. In order to improve the bioavailability of KTZ we obtained a new formulation with PAMAM dendrimer G5. The supramolecular assembly was confirmed and characterized by XRPD, DSC and FTIR techniques. The in vitro release profile of the encapsulated KTZ by the dialysis method in water was also determined. The biocompatibility was assessed by the MTS assay in the hepatic cell line HepG2 and shows similar results for G5-PAMAM and KTZ-G5, with the cell viability above the toxicity limit. The risk for allergy induction following cutaneous exposure to KTZ-G5 was tested by the mouse ear swelling test and shows a negative result, similar to the negative control. All the results sustain the improvement of KTZ properties making the new supramolecular Ketoconazole-PAMAM dendrimer carrier system an interesting candidate for developing topical dosage formulation of enhanced bioavailability and therapeutic effect.

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Poster T2-20

Structural study of cataract-causing p23T mutant of γD-crystallin by Nuclear Magnetic Resonance

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Abstract. Cataract is a major cause of blindness worldwide, either because of age-related degenerative modifications, or genetic mutations, causing abnormal aggregation of eye lens crystallins. While age-related cataracts occur only in adults, inherited congenital cataracts manifest in early childhood. Currently the only effective treatment for cataract is surgery, without any possibility of prevention. A complete elucidation of the molecular mechanism of crystallin aggregation is essential for understanding cataract formation. In this study, we investigate the molecular aggregation pathway of the Pro23Thr mutation in γD–crystalline isotopically ^{15}N-labeled, using Nuclear Magnetic Resonance. We are exploring alternatives, screening for potential inhibitors interfering with the phase-separation mechanism, followed by *in vitro* assays against hγD-P23T aggregation.

Poster T2-21

Inclusion of CHT in β-cyclodextrin nanocavity and its effect on antioxidant potential of CHT: A calorimetric, spectroscopic and molecular docking approach

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Abstract. The inclusion complex formation of CHT and β-cyclodextrin in aqueous solution has been investigated using ITC, spectroscopic and theoretical methods. The stoichiometry of this inclusion complex was established to be equimolar (1:1) and its equilibrium constant was determined. Our observations also that hydrophobic interactions are the key interactions that prevail in the complex. ^{1}H NMR spectroscopic method was employed to study the inclusion process in aqueous solution. Job plots derived from the ^{1}H NMR spectral data demonstrated 1:1 stoichiometry of the inclusion complex in liquid state. 2D NMR spectrum suggest the orientation of the aromatic ring of CHT inside β-CD cavity. The antiradical activity of the complex was evaluated and compared with free CHT, indicating a delayed activity compared with free CHT. To obtain an additional qualitative and visual insight into the particularity of CHT and β-CD interaction, molecular docking calculations have been performed.

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Poster T2-22

Structural changes of bacterial strains DNAs upon femtosecond laser irradiation, as proved by Fourier transform infrared (FT-IR) spectroscopy

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Abstract. In this work, the effects of femtosecond laser pulses irradiation time, femtosecond laser pulses treatment wavelength and strain type, respectively, on the structure of bacterial DNAs is presented, by using Fourier transform infrared (FT-IR) spectroscopy. Several sets of irradiation parameters are considered for DNAs from two bacterial strains, respectively. Fourier transform infrared spectra of genomic nucleic acids have been discussed for control and irradiated samples, respectively. FT-IR absorbances assignments and structural behavior of DNA subgroups are analyzed in the 800-1800 cm^{-1} spectral interval.

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Poster T2-23

Effect of focusing on SERS spectra profiles studied by experiment and FDTD simulation

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Abstract. The effects of objective numerical aperture and focusing of the laser beam on the SERS signal of 4-aminobenzenethiol Raman reporter molecules adsorbed on gold film over nanospheres (AuFoN) substrates are investigated. Upon in-depth analysis of sequential spectra within z-axis linescans, we observed that the position of the focal point of the incident laser beam relative to the AuFoN surface has a significant, not only quantitative, but also qualitative impact: the shape of the recorded SERS spectra can be considerably modified. FDTD simulations performed on realistic 3D model suggest that the observed effect can be induced by the spectral distribution of the plasmon-enhanced near-fields, which can be modified by focusing. These observations can have a significant impact on the way SERS spectra are processed and band ratios or molecular concentrations are calculated, and thus, are relevant for various analytical applications.

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Poster T2-24

Antioxidant Activity Evaluation and Assessment of the Binding Affinity to HSA of a New Catechol Hydrazinyl-Thiazole Derivative

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Abstract. Polyphenols have attained pronounced attention due to their ability to provide numerous health benefits and prevent several chronic diseases. In this study, we designed, synthesized and analyzed a water-soluble molecule presenting a good antioxidant activity, namely catechol hydrazinyl-thiazole (CHT). This molecule contains 3',4'-dihydroxyphenyl and 2-hydrazinyl-4-methyl-thiazole moieties linked through a hydrazone group with very good antioxidant activity in the in vitro evaluations performed. In this paper, we report the binding mechanism of CHT to HSA using biophysical methods in combination with computational studies. ITC experiments reveal that the dominant forces in the binding mechanism are involved in the hydrogen bond or van der Waals interactions and that the binding was an enthalpy-driven process. NMR relaxation measurements were applied to study the CHT–protein interaction by changing the drug concentration in the solution. A molecular docking study added an additional insight to the experimental ITC and NMR analysis regarding the binding conformation of CHT to HSA.

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Poster T2-25

Determination of pesticides residues in eggplants using gas chromatography-mass spectrometry

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Abstract. Pesticides are intensively used in vegetables production, but they manifest negative effects on consumers health. The application of fertilizers and implicitly pesticides, combined with other external polluting factors, specific to the geographical region of agricultural crops, significantly affects the content of some mineral elements in the soil, the plant and subsequently the finished product, which is why the development and implementation of a system of traceability, at the national level, on the path "from the farm to the fork" becomes a necessity. This study presents the investigation of 63 pesticides in 5 samples of eggplants from 5 different areas by gas chromatography-mass spectrometry (GC-MS). The GC-MS analysis was performed using an Shimadzu Nexim 2030 gas chromatograph mass spectrometer, at a temperature of the ionization source of 230°C, ionization mode: EI, 70 eV, using two columns, Column1 - Rxi-MS (60mx0.25mmx0.25µm), the injector at 260°C, carrier gas-helium with a flow of 1L/min, injection volume -1µL, and an analysis time of 48 minutes. Multiple pesticides residues were detected in all samples. Seven pesticides (atrazine, boscalid, carbofuran, chloropyrifos, cyprodinil, pirimicarb and tebuconazole) were detected in the analysed samples with concentration range between 0.02-0.09 mg/kg. It is concluded that the continuous monitoring and strict regulation of pesticide use on food crops, especially vegetables, are necessary. **Acknowledgments.** The work has been conducted under Sectorial Plan-ADER 2026, Project ADER 6.3.7 – "Applicability measures regarding the investigation of the organochlorine and organophosphorus contaminants distribution on the soil-plant-vegetable/fruit-finished product chain, following different types of soils in various areas", financed by Ministry of Agriculture and Rural Development - Romania and NUCLEU Program-Financing Contract no. 20N/05.01.2023, Project PN 23 15 03 01, financed by the Romanian Ministry of Research Innovation and Digitalization.

Poster T2-26

EPR fingerprinting of yeast cells overexpressing metal-binding peptides

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Abstract. This work aims to develop an efficient and reliable method to monitor intracellular proteins by Electron Paramagnetic Resonance (EPR) spectroscopy. For this purpose, a cellular model expressing Green Fluorescence Protein (GFP) tagged with an array of metal-binding oligopeptides (MeBPep) designed to trap EPR-responsive metal ions, such as Mn(II) or Cu(II) is used. This model develops EPR spectroscopy as a toolbox for comparative profiling of cells – both standard and expressing metal-binding peptides - in the absence or the presence of heavy metals, both essential and not essential for life. Starting from the observation that some strains expressing GFP-MeBPep hyperaccumulated Mn(II) or Cu(II) resulted from metal sequestration by MeBPep, we tested if such MeBPep could be used to trap EPR-active cations for the analysis of MeBPep-tagged proteins by EPR.

Poster T2-27

Spectroscopic NMR and FT-IR approach used for the evaluation of healing after surgical interventions for patients with Colorectal Cancer

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Abstract. Worldwide, the colorectal cancer (CRC) is one of the most common and deadly types of cancer. Compared with the time consuming of the classical histopathological approach, this study discusses the application of ^{1}H NMR and FT-IR spectroscopic techniques for the fast evaluation of healing degree of patients with CRC after surgical intervention. For that, blood plasma, native, deproteinized and proteins from plasma were analysed for a number of ten patients with confirmed CRC and ten healthy volunteers. Plasma samples collected from CRC patients present higher lipid and protein content compared to healthy controls, as was detected by FT-IR and ^{1}H NMR spectroscopy. Moreover, ^{1}H NMR relaxometry was used to measure the proton mobility which reflects changes in plasma composition and structure associated with CRC. Finally, the most relevant parameters were included into a Principal Component Analysis (PCA) test. For that, the main classes are represented by the parameters measured for the samples collected from CRC patients before intervention, after intervention (at 7 days) and healthy patients. The results are systematically classified using a trained Artificial Neuronal Network (ANN) based on machine learning (ml5) library. The healing degree is then evaluated by ANN using the regression method. In conclusion, various techniques (experimental NMR and FT-IR and numeric ML) were combined to evaluate the patient healthy state.

Poster T2-28

Cross-polarization under fast MAS NMR: from spin dynamics to experimental methods

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Abstract. Investigation of low natural abundance nuclei (e.g. ^{13}C, ^{15}N) by solid-state NMR requires the use of the cross-polarization (CP) under magic-angle spinning (MAS) for transferring the polarization from the high natural abundance and faster relaxing ^{1}H nuclei. However, the higher the spinning frequency, the worse the CP efficiency. As many modern applications on complex (bio)molecular systems rely on fast MAS (> 50 kHz), there is a need to understand the polarization transfer process also at high rotation frequencies, and to improve its efficiency. Here, we analyze the spin dynamics in the cross-polarization process for different spinning frequencies, from 20 kHz to 60 kHz, by numerical simulations and experiments. For this purpose, the changes in the polarization transfer time (τ_{CP}), relaxation in the rotating frame ($T_{1\rho}$), and the exchange phenomena, respectively, with respect to the increase of the spinning frequency have been investigated. Based on these results, possible methods to obtain better cross-polarization efficiency under fast MAS NMR conditions are discussed.

Poster T2-29

Oxidative stress evaluation in cells exposed to halloysite nanoparticles

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Abstract. Several types of cells belonging to HaCaT, BJ, A375, A549 lines have been exposed to halloysite nanoparticles (NP) in order to investigate the possible cytotoxic effects. With regard to oxidative stress, two different strategies have been performed: the enzymatic (SOD, CAT) determinations and the non-enzymatic pathways regarding the concentrations of TAC, TOS and oxidative stress index estimation. Therefore, the results emphasize the sensitivity of some cells when exposed to NP, whereas other types of cells are more resistant to the same NP concentration. By far, HaCaT cells were more resistant and did not present any particular changes in the oxidative status after exposure to NPs, neither the SOD and CAT activities presented significant changes. The most vulnerable and sensitive of all cell types, according to our studies, were the A375 cell line, melanocytes, in which the plasma membrane suffered significant changes after the exposure to halloysite nanoparticles.

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Poster T2-30

Competitive oligomer-protein aptamer interaction for target quantification *via* SERS/SEF mechanism

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Abstract. Surface-Enhanced Raman Scattering (SERS) and Surface-Enhanced Fluorescence (SEF) are powerful spectroscopic tools for the detection of scant amounts of specific molecules. Due to their exceptional optical properties, plasmonic nanoparticles are often used to produce surface enhanced-active substrates with reproducible and robust signals to be employed in the development of optical molecular sensors. Herein, we propose a SERS/SEF biosensor based on Epidermal Growth Factor Receptor (EGFR)-specific aptamer conjugated gold nanoparticles that can be exploited in liquid, as colloidal suspensions, or as films deposited onto solid substrates. We studied the competitive interaction of a complementary short sequence oligomer tagged with the ATTO-647N fluorophore *versus* the EGFR protein by monitoring the SERS/SEF signal of the fluorophore as it interacts with the plasmonic nanoparticle surface.

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Poster T2-31

Plasmonic structural colours *via* metal-coated colloidal microsphere arrays

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Abstract. Structural colouring based on plasmonic nanostructures exploits the interaction of light with nanostructured metallic surfaces, resulting in selective reflection/transmission of certain spectral ranges of the visible domain. Unlike traditional pigments that absorb light based on their chemical composition, plasmonic nanostructures rely on their physical structure to achieve colours. Here we explore the possibility of obtaining colours by using self-assembled colloidal microsphere lattices coated by thin metal films. By using Finite-Difference Time-Domain (FDTD) simulations on realistic models we explore the optical reflectance of dielectric microsphere lattices of various sizes (300-700 nm) coated by different metal (Al, Ag, Au) films of various thicknesses (20-200 nm). Reflectance spectra are then converted into their specific colour by using a Matlab software algorithm. Next, to prove the feasibility of the concept, several Au-coated and Ag-coated two-dimensional polystyrene microsphere arrays are fabricated and their reflectance spectra and colour images recorded. The obtained plasmonic colours are tuneable by sphere size and metal material and its thickness, making them a promising tool for developing new colour-based applications.

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Poster T2-32

High order harmonic generation in modulated waveguides

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Abstract. High order harmonic generation (HHG) in dielectric waveguides (WG) modulated in size is explored via numerical simulations. The IR (800 nm) and mid-IR (2000 nm) femtosecond pulses are considered and the electric field space-time configuration in such structures is first found using a split-step method adapted for high ionization of the gas medium inside the WG. The variation of the WG diameter induce a variation of the driving field intensity and phase, which is different from the straight WG case, and induce a different phase matching regime in the HHG process. An amplification effect in harmonic intensity is seen at very high orders generated by the mid-IR radiation, and the possibility to obtain soft X-rays in the water window range is analysed.

Poster T2-33

Ultrashort laser pulse characterization by deep learning methods

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Abstract. SHG-FROG (Second Harmonic Generation - Frequency Resolved Optical Gating) can be used for a complete characterization of ultrashort laser pulses. In a SHG-FROG measurement a spectrogram image is recorded, from which the amplitude and phase can be recovered by different inversion algorithms. In the present work we present a pulse retrieval method, based on deep convolutional neural networks, with the aim to be faster than classical algorithms. We train the neural network on computationally generated FROG images and generate our dataset by a semi-empirical method, where the spectral phase is calculated through its Taylor expansion, using parameters like the grating distance or incident angle of a laser system. Our results show a good and fast reconstruction of the simulated laser pulses with low values of the reconstruction error on a test set.

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Poster T2-34

Adhesion of Short Antimicrobial Peptides to Bacterial and Mammalian Membrane Models – A Molecular Modeling Approach

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Abstract. Wound healing is considered a dynamic and complex process. Therefore, an appropriate diagnosis and optimal wound dressing are essential to ensure proper healing. A shift towards the use of short (below 50aa) antimicrobial peptides (AMPs) that exhibit activity against drug-resistant bacteria has been reported in recent years. AMPs are part of the host innate defense mechanisms of many eukaryotic organisms, most of which are amphipathic and cationic peptides (with a net charge from +2 and +7 at physiological pH). Here we present preliminary results using *in silico* methods on the adhesion to bacterial and mammalian membrane models (DOPC+DOPG 85:15, and DOPC, respectively) of histidine modulated arginine- and tryptophan-based short AMPs (RW-AMP) that will be used in designing AMP-functionalized smart wound patches. Hence, we used (i) molecular dynamics to assess AMP's adhesion times, and (ii) potential of mean force calculations to determine binding free energies. Our results suggest more stable binding and stronger adhesion of RW-AMPs to bacterial membranes vs. mammalian membrane models. Moreover, the RW-AMPs closer positioning to the PG groups of the bacterial membrane model leads to increased interaction with the DOPC headgroups.

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Poster T2-35

Rapid determination of total iodine in solid samples using HPTLC method

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Abstract. Iodine is an essential micronutrient for humans and animals. Since inadequate iodine intake in diets leads to the risk of developing several health disorders, development and validation of reliable analytical methods for quantitative evaluation of iodine in samples such as food, dietary supplements and pharmaceuticals are justified. In contrast with other elemental analysis, iodine determination imposes real challenges regarding sample preparation due to its volatility but also due to analytical technique limitations since standard ICP-OES and AAS spectrometric techniques are usually not performant enough. Either very expensive techniques such as ICP-MS or classic kinetic colorimetric Sandell-Kolthoff method are usually employed for ordinary iodine analysis. In this work, we present a simple and unique chromatographic method for iodine determination based on chromatographic evaluation of the tyrosine iodination using HPTLC. Samples are mineralized via oxygen combustion procedure and the so formed iodide-containing solution is used to iodinate tyrosine by the action of a specific oxidant. Unreacted tyrosine and iodinated tyrosine are extracted via a solid phase extraction cartridge and the collected analytes are simply analysed on HPTLC silica gel plates. The mobile phase is optimized using response surface methodology and the method is applied for the analysis of real samples.

Poster T2-36

Microfluidic integration of electrochemical surface-enhanced raman scattering sensors for detection of pesticides in surface waters

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Abstract. Our ecosystem suffers from pesticides and their residues that make their way into aquatic media compromising supply of safe and clean drinking water and the public health. This work reports on the microfluidic integration of sensors based on Surface-enhanced Raman scattering (SERS), optionally coupled with electrochemical (EC) sensing, i.e., EC-SERS for the sensitive detection of pesticides in water. In this contribution, we summarize findings from the on-going project POLSENS. This project addresses the existing technological gap in the development of portable sensors for determination of pesticides in surface waters in real time. Four types of sensors have been investigated: i) electrochemically activated and roughened commercial screen-printed electrode (SPEs), ii) microfabricated thin film TiW-Au electrode, (iii) nanopatterned Au-metallized nanoimprint resist, and iv) Au-metallized polysterene (PS) nanospheres deposited using colloidal self-assembly. We compare several approaches for SERS and EC-SERS sensors fabrication and microfluidic integration, crucial for sensitive detection of pesticide molecules. Detection of thiobendazole, fungicide often used to control diseases in a wide range of crops, is a relevant application case used to compare the performance of sensors. The lowest detectable concentration is currently 10-7 M. We envision that the limit of detection can be improved and discuss the factors influencing it.

SECTION T3

Green Energy and Innovative Technologies

Oral T3-1

Optimizing the properties of cement composites for 3D printing via NMR relaxometry

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Abstract. 3D printing technology has the potential to significantly decrease the environmental impact of cement-based materials, particularly by a better exploitation. An advantageous aspect of constructing buildings without traditional formworks is the ability to save on costs, time, and materials that are typically associated with formwork construction. Furthermore, this approach allows for the design and realization of more intricate structures. However, to fully replace the functions usually fulfilled by formworks, it becomes essential to develop novel cement-based composites that exhibit rapid setting and low slump characteristics. The addition of accelerators, silica fume, and metakaolin allows the control of hardening rate. Therefore, understanding the influence of all these additives on hydration dynamics and pore evolution becomes crucial for achieving the desired properties of cement-based composites. In our research, we employed low-field nuclear magnetic resonance (NMR) relaxometry to monitor the impact of varying the proportion of these additives on dormancy stage, the evolution of pore size, and changes in internal surface properties. The findings from NMR relaxometry investigations were correlated with the sample strength and the setting time.

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Oral T3-2

Vibrational contributions to electrochemical potential of MOF electrodes

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Abstract. We present a theoretical study of the vibrational contributions to electrochemical potential of organic electrodes in Li-ion batteries. The vibrational energy contribution to Nernst equation is calculated using the DFT and molecular dynamics. For each oxidation state (i.e. number of Li ions in the structure) we evaluate the vibrational density of states and the electrochemical potentials associated to it (entropy, energy and free energy). Out results indicate a strong dependence of vibrational contributions on the oxidation state as well as a relatively important contribution to the total electrochemical potential. We show that a fine-tuning of these contribution is possible by a specific design of the geometric structure of organic electrodes at nanoscopic scale.

Acknowledgements. The authors acknowledge financial support from UEFISCDI Romania, project PN-III-P4-ID-PCE-2020-0824.

Oral T3-3

Power supply sharing for energy accumulation home appliances: the good and the bad - preliminary data

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Abstract. A household appliance with energy accumulation is able to store thermal energy for further use. This allows the sharing the power supply of these devices in two phases: accumulation and consumption. Once the energy accumulation has stopped, the stored energy into device is consumed until the new accumulation phase occurs. The two phases may follow each other indefinitely. We present a simple method of sharing the power supply without negative effects in the operation of these types of devices, which achieves an energy saving of about 50%. The tests were conducted during 6 months on two common refrigerators by implementing electrical energy measurement (energy meters connected via MODBUS interface to a laptop) and internal temperature/humidity measurements (data-logger). Based on the preliminary measurements we can conclude: the method is suitable for power supply sharing in both off-grid and on-grid networks. In an off-grid network a 13% increase of SoC after 12h of continuous discharge of a power-wall (7kw, LiFePo4) was achieved by power supply sharing. Some secondary issues caused by the power switching were corrected using suitable filtering devices. Further work is necessary to implement the method in an embedded system controlling all similar appliances connected to an off-grid network with limited input power. A patent request for the method and for a device supporting the method was issued.

Oral T3-4

Let's help improve public health: meet our innovative cold plasma disinfection systems

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Abstract. Given the situation on the Planet with the last case of large scale pandemic, we as scientists have to definitely do our best to help with whatever we know and can do, to assist in the global effort to minimize the effects of pathogenic microorganisms. This main motivation is doubled by the fact that most of our beloved ones/relatives were affected at some point by pathogenic microorganisms in one way or another, either physically, emotionally, socially or economically. As it is quite well known already, the virions remain viable on various surfaces (plastic, metals, synthetics, etc.) for several hours. This presents a transmission cycle for human infection that can be interrupted by developing new inactivation devices and technologies. Various virus inactivation methods are used to prevent viral spread in different matrices, but unfortunately so far the ideal method has yet to be discovered. Each of the currently used decontamination methods (especially the chemical ones) present drawbacks. Cold plasma has entered this field as a novel, highly efficient and clean solution for virus inactivation. Cold atmospheric plasma (also known as open-air non-thermal plasma) operating at atmospheric pressure and almost room temperature (T<45 deg.C), has been shown to safely and effectively treat contaminated surfaces and can treat both smooth and rough surfaces. Among its complex constituents, the emission of UV radiation and reactive oxygen and nitrogen species have the most important antimicrobial properties. UV photons damage nucleic acids, whereas the highy reactive molecular species present in the plasma can oxidize the viral nucleic acids, proteins and lipids. Our research team presents here three plasma disinfecting systems which we designed and built, systems that can definitely help in the disinfection processes:

1) An automatic hand plasma cleaner/disinfecting system
2) A bus handle bar plasma cleaner/disinfecting device
3) A floor and wall plasma disinfecting machine designed for use in hospitals.

Oral T3-5

Building better superconducting qubits

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Abstract. Superconducting qubits have emerged as the most promising platform for scalable quantum computers. Despite the successes and the popularity of superconducting qubits, there are still many roadblocks that prevent the scaling of quantum processors beyond one hundred of connected quantum bits. We present our work on qubit modelling and noise mitigation in the broader context of the research done by the superconducting quantum computing community for improving the quality of these qubits.

Oral T3-6

The Development of simultaneous XAS and XRD measurements 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 catalysis reaction mechanisms in nanoparticles, the phase change 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, simultaneous X-ray absorption spectroscopy and X-ray diffraction characterization techniques, are used in the investigating complex systems. Using several representative examples, we illustrate the role of simultaneous techniques in the characterization of new details about the degradation process of organic-inorganic hybrid perovskite, the catalytic reaction mechanisms of nanoparticles, and also the phase change of novel materials. Following these approach it is possible to design and prepare novel materials.

Poster T3-1

Simulations of the combustion process with different hydrogen/methane mixtures

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Abstract. The high interest in increasing energy production at a global level combined with the need to reduce pollution has led to the development and growth of energy production from alternative sources (solar, wind, etc.). The energy production from these sources has the disadvantage that it is not constant and thus the need to store it arises. Storing excess solar and wind energy in the form of hydrogen to be injected into the national natural gas grid is considered an important step in the energy transition. Previous research has shown that it is possible to inject hydrogen into the natural gas network, up to a molar concentration of about 50% without affecting the functionality of end-user devices. The technical solution refers to the optimization of the combustion process for different H_2-CH_4 mixtures for the Genoa 03 Stirling engine coupled with a 3 kW electric generator. The geometric model was discretized based on the finite element theory and then the physical models were chosen from the Ansys Fluent module: Energy, realizable k-ε turbulent model, Non-premixed combustion (with stoichiometric combustion). The fuel flow rate used in the simulation was the one determined experimentally as necessary for the operation of the Stirling engine 0.00032kg/s. CFD simulations were performed for mass concentrations of 0, 5, 10 and 15% hydrogen in methane. Air flow was calculated consistent with stoichiometric combustion. It should be noted that a mass concentration of 10% H_2 is equivalent to a molar concentration of 46.9% H_2. Based on the results of the CFD simulations, both the power lost (stored in the flue gases) and the power absorbed by the heat exchangers of the Stirling engine were calculated. In conclusion, the implementation of the technical solution presented in this phase can have a beneficial effect both by reducing the amount of fuel needed to operate the Stirling engine and by reducing the emissions of carbon dioxide released into the atmosphere, without affecting the functionality of the engine.

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Poster T3-2

Efficient generator design for low wind turbines

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Abstract. Wind energy is one of the most exploited sources of renewable energy nowadays. There are numerous types of wind turbines and windmills that use blades in order to catch the wind energy and convert it into electricity. Most wind turbines are installed on land or in places where wind corridors exist. Even though large-scale wind turbines are highly used, low wind turbines are more challenging due to the unpredictable wind speed and due to the electronic design of the switching circuit. This work is focused on the design of an efficient generator for low wind turbines. The numerical analysis is performed in COMSOL Multiphysics software. Different approaches regarding the type and number of magnets, pole number and coils have been considered.

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Poster T3-3

Computational assessment of Al-based materials

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Abstract. In material manufacturing it is usually impossible to discriminate between the role and weight of each factor that may affect the structure composition at nanoscopic scale. This gap can be filled by computational modeling techniques and methods. One of the most powerful is the molecular dynamics (MD), which provides detailed information on the effect of substitutional disorder, defects, vacancies, pressure or temperature onto the manufacturing process, and allows to isolate and control the parameters and conditions for manufacturing.

We will present here our data on Al2O3 and grAl structures that resulted from the QuCos project activities.

Acknowledgements. This work is supported by UEFISCDI Romania through the project Quantum Computation with Schrödinger cat states, contract ERANET-QUANTERA-QuCos 120/16.09.2019

Poster T3-4

Wind and Hydrogen-Based Hybrid Power System for a Passive House. A Case Study

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Abstract. The present case study approaches the optimal sizing design of a wind and hydrogen-based hybrid power system for a passive house in Râmnicu-Vâlcea, Romania. The designed hybrid energy system guarantees uninterrupted and reliable power for the proposed building throughout the year. The hybrid energy system uses wind speed as the primary renewable resource of power generation and hydrogen delivered through a hypothetical centralized distribution network, converted into electricity by means of a fuel cell stack, as a secondary energy resource. The analysis of this type of hybrid power system was carried out to meet the perspective of the future hydrogen-based economy, which assumes that there will be a hydrogen transport and distribution network. Since the reliability of the electricity supply is critical for the passive house, optimal sizing of the energy conversion equipment, wind turbine, and fuel cell stack, but also the hydrogen storage tank is essential. The studied passive house type building has an estimated electricity annual consumption of 5070 kWh, and the optimally sizing hybrid power system has the main equipment components: DC Southwest: Whisper 500 wind turbine with a capacity of 3260 W at a wind speed of 14 m/s, fuel cell with nominal power of 2 kW, 1800 VA inverter and storage tank for a maximum of 10 kg of hydrogen. During one year of power system operation, the wind turbine produced 49.11% of the total electricity generated by the studied system, and the fuel cell provided electricity for the analysed building of 50.89%. The passive house energetically supported by the studied hybrid power system generates carbon dioxide emissions embedded in the system in the amount of 0.06 kgCO_2/kWh, which represents 19.64% of the average value calculated for a standard building energetically supported by classic power systems based on conventional fossil resources.
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Poster T3-5

Towards eco-sustainable aluminum-air batteries

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Abstract. Aluminium-air batteries are energy conversion devices considered promising alternative to lithium-ion batteries. This is due to their high theoretical energy density which results from the coupling of a metal anode and a catalysed cathode with an open structure that allows reactions with atmospheric oxygen. In addition, aluminium is one of the most abundant element on the Earth's crust and its recycling chain is well proven. The use of water-based electrolytes and raw materials of natural or synthetic but biodegradable origin in the battery components, mainly electrolytes and cathodes, adds the further advantage of safety, affordable cost and eco-friendliness. In this work, the electrochemical performances of Aluminum-air batteries assembled with aqueous polymer electrolytes made with natural polysaccharides are investigated and discussed, by comparing the results obtained by using cathodes based on platinum catalyst with respect to a cheaper wood-derived activated carbon. Three-electrode discharge measurements, rate performance tests and linear sweep voltammetry were used to critically compare different cathodic materials. The results show that the best electrochemical performances are obtained for Al-air cells assembled with wood-derived air cathodes.

Poster T3-6

Effect of Sr^{2+} ions on the physical, optical and structural features on molybdenum-copper-lead glass

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Abstract. In this study, the structural properties of a glass system with varying compositions of SrO-MoO_3-CuO-PbO_2 were investigated using Fourier Transform Infrared (FTIR) and Ultraviolet-Visible (UV-VIS) spectroscopic techniques. The glasses were prepared through the melt-quenching method, and their physical properties such as density and molar volume were determined. The effect of SrO concentration on the endothermic and exothermic processes was studied using Differential Scanning Calorimetry (DSC). The gamma photon shielding ability of the glass samples in the photon energy range of 0.15–15 MeV was calculated theoretically. The results showed that the addition of SrO to the glass matrix increased its density, reduced the molar volume, and enhanced its thermal stability. The UV-VIS spectra indicated the presence of non-bridge oxygens at high Sr2+ ion concentrations, leading to an increase in defect states and the degree of disorder in the glass structure, resulting in a decrease in the optical band gap energy. The FTIR spectra revealed the formation of isolated $[MoO_4]^{2-}$ anions at high SrO concentrations, which negatively affected the glass forming ability, in agreement with the thermal analysis data. The physical, optical, and structural properties of the molybdenum-copper-lead glass were found to strongly depend on the SrO content.

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Poster T3-7

CFD Simulation and Comparative Analysis of Three Liquid Metal Based Solar Reciever Designs: Enhancing Efficiency and Performance

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Abstract. The main goal of this study is to realize computational fluid dynamics (CFD) simulation of three distinct types of solar recievers used in concentrated solar power systems. The study is based on some previous results obtained from an optical simulation software, that provides energy distribution type results as well. The objective is to evaluate and compare the performance and efficiency of these recievers. The CFD simulations were conducted to analyze the flow behavior, heat transfer characteristics, and thermal performance of each solar reciever. The simulations considered the effects of geometry and placing isolating layers on the receiver on the overall efficiency. The work fluid is a liquid metal with low melting point and good thermal conductivity.

Through a comparative analysis, the study highlights the strengths and weaknesses of each reciever design in terms of efficiency, temperature distribution, heat transfer but also the complexity of the design. This research contributes to the optimization of solar energy systems by providing valuable information for the selection and design of solar recievers suitable for specific applications.

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Poster T3-8

Valorization of Agro-Industrial Residues through the Production of bioproducts with added value in the circular bioeconomy system

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Abstract: The agro-industrial sector generates significant amounts of residues, most of them not being properly processed, and thus becoming a threat to the population and the environment. Thus, cascade valorization of agro-industrial plant biomass (APB), through the transformation into bioproducts, with closing the value loop in the economy, shows an increasing interest nowadays. This work aimed to present the state of the art related to the transformation of APB (*eg.* fruit pomace and forest industry waste) into: (i) high value products with therapeutic potential (bioactive phytochemical extracts and pectin) to ensure the food and nutritional security of the population; (ii) bioethanol with applicability in bioeconomy and biofuel; (iii) biohydrogen, biomethane, hytan as biofuels and energy vectors; (iv) biofertilizers to improve soil quality and a transition to organic agriculture. Environmentally friendly materials (microorganisms, enzymes, bacteria) and methods (microwave extraction, ultrasound field extraction, enzymatic hydrolysis, microbial fermentation) will be considered in order to support the transition to green energy and a clean environment for a healthy population based on efficient use of natural resources, with the closure of the value chain and supporting the concept of almost zero resulting waste.

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Poster T3-9

From green to white analytical chemistry: concepts and simple laboratory examples

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Abstract. In pursuance of environment protection and human safety, green analytical approaches are preferred over classical procedures. Whereas the greenness of an analytical methods is an important aspect, its usefulness and proper functionality is the core track during their development. The concept that combines both, the analytical efficiency and practical/economical aspects is that of *white* analytical chemistry. In the last two decades, numerous metric tools were developed in order to evaluate the greenness degree of an analytical method, whiteness level are still novel approaches but highly welcome in the field of analytical chemistry. This work aims to show some specific laboratory examples of analytical approaches as greener and whiter alternatives to the classic ones. They will include greener and whiter sample preparation for selenium analysis based on both fluorescence spectroscopy and cyclic voltammetry. Whereas classic sample preparation for selenium analysis involves highly concentrated mineral acids, our step is not only fast but is based on a straightforward and fast catalytic combustion in molecular oxygen rich atmosphere. In addition, simple sample reduction in classical qualitative analysis is advocated as not only eco-friendly approach but also more efficient for the evaluation of analytical performance evaluation such as limit of identification of classic analytes.

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Poster T3-10

Super drawer testing and certification

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Abstract. The Super-Drawer assembly will be tested for certification before installation in the Tile Calorimeter modules using a custom test bench consisting of: (i) Long Black Box (LBB) - 3m long light tight enclosure that reproduces the interior of the TileCal girder (with girder rings and optical fibers), (ii) three meters Long Basket (LB) for entire SD extraction in case of a PMT block replacement and (iii) Prometeo - standalone readout system.

Poster T3-11

Solar Heating Simulation and Comparative Analysis of Three Liquid Metal Based Solar Receptor Designs: Enhancing Efficiency and Performance

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Abstract. Prior to conducting computational fluid dynamics (CFD) simulations for the purpose of acquiring valuable information regarding heat exchange in three distinct types of solar receptors and subsequently determining the most suitable receptor for solar energy conversion applications, it is necessary to obtain the radiation distribution across the receptors surfaces.

By utilizing a ray tracing program, each solar receptor was incorporated into an optical system comprising a radiation source and a Fresnel lens. The solar radiation source was configured to generate an equivalent total flux across all three cases while encompassing three predominant weighted wavelengths. Distinct optical properties were assigned to the receptor surfaces, taking into account their absorbance, reflectance, and insulating characteristics. The outcomes facilitated minor adjustments aimed at enhancing the design of each receptor and yielded significant insights to inform subsequent CFD simulations.

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Poster T3-12

Optimization of the electrothermal evaporation process based on intelligent control of the power source

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Abstract. Electrothermal evaporation in the electrothermal vaporization capacitively coupled plasma optical emission spectroscopy (ETV-µCCP-OES) systems is a key element and the optimization of the drying and vaporization temperature has a major impact on the measurement process and the accuracy of the results obtained. In the present research, the use of a power source with digital control was pursued and, using a Labview interface, an intelligent algorithm was developed for the optimal control of the exposure time and the temperature thresholds at which the drying and vaporization process takes place. Testing was performed on standard solutions with known concentrations of Cd and Zn. The obtained results show that through the intelligent control of the drying and evaporation stages in terms of times and temperature thresholds, the accuracy can be improved by up to 20% compared to the classic manual control of the power source. At the same time, the repeatability of the measurements is significantly improved and the energy consumption is minimized. Process optimization is intended to continue towards integration into a complete intelligent control loop, including other process control parameters such as argon flow and spectra recording.

Poster T3-13

Exploring the terrain of noise in superconducting qubits

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Abstract. Superconducting circuits are one of the most successful approach for developing qubits due to their flexibility in customizing their Hamiltonian. There are several ways to improve a superconducting qubit like material refining and circuit parameter optimization. We study the interaction of different qubit architectures to the environment and we determine how quantities such as anharmonicity, dispersive shifts and decoherence rates depend on the physical parameters of their circuit elements.

Poster T3-14

Add-on sensors for photovoltaic panels

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Abstract. Photovoltaic (PV) panels convert solar energy into electrical energy and the conversion process is negatively influenced by the rise of the temperature of the panel. This poster presents the concept of an add-on sensory platform that can be attached on commercially available (photovoltaic) PV panels. The sensory platform is meant to collect and transmit data from on-board sensors, from the temperature sensor attached on the non-irradiated (back) side of the PV panel and from an energy measurement module. Hence, the platform measures the energy drawn from the PV panel, the temperature of the panel and the intensity of the incident light. The sensory platform is able to store locally acquired data. A wireless module, contained by the platform, enables the platform to send data through LoRa communication.

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Poster T3-15

Solar and Hydrogen-Based Hybrid Power System for a Passive House. A Case Study

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Abstract. The present case study approaches the optimal sizing design of a solar irradiation and hydrogen-based hybrid power system for a passive house in Râmnicu-Vâlcea, Romania. The designed hybrid energy system guarantees uninterrupted and reliable power for the proposed building throughout the year. The hybrid energy system uses solar irradiation as the primary renewable resource of power generation and hydrogen delivered through a hypothetical centralized distribution network, converted into electricity by means of a fuel cell stack, as a secondary energy resource. The analysis of this type of hybrid power system was carried out to meet the perspective of the future hydrogen-based economy, which assumes that there will be a hydrogen transport and distribution network. Since the reliability of the electricity supply is critical for the passive house, optimal sizing of the energy conversion equipment, photovoltaic (PV) panels, and fuel cell stack, but also the hydrogen storage tank is essential. The studied passive house type building has an estimated electricity annual consumption of 5070 kWh, and the optimally sizing hybrid power system has the main equipment components: 22 photovoltaic panels with a total installed nominal power of 6.16 kW, fuel cell with nominal power of 2 kW, 1800 VA inverter and storage tank for a maximum of 10 kg of hydrogen. During one year of power system operation, the photovoltaic panels produced 66.14% of the total electricity generated by the studied system, and the fuel cell provided electricity for the analysed building of 33.86%. The passive house energetically supported by the studied hybrid power system generates carbon dioxide emissions embedded in the system in the amount of 0.05 $kgCO_2$/kWh, which represents 16.36% of the average value calculated for a standard building energetically supported by classic power systems based on conventional fossil resources. **Acknowledgements.** This work is supported by MCID Romania, Project PN 23 15 01 01, Contract No. 19PFE/30.12.2021 and a grant of the National Center for Hydrogen and Fuel Cells (CNHPC)—Installations and Special Objectives of National Interest (IOSIN).

Poster T3-16

Properties of waste modified bituminous mastic

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Abstract. Recirculating materials by using them more efficiently in new products, and increasing their utilization and lifetime could significantly reduce demand for primary industrial materials and thus reduce environmental impacts. In this context we present the preparation of a new composite material as an alternative to the commercial filler, which is a non-renewable resource, used to prepare bituminous mastic with significant applications in the construction industry. The composite material is based on two industrial wastes: stone dust and waste cooking oil. Several bituminous mastic compositions were tested at laboratory level and compared to the corresponding standard requirements for commercial products by determining the thermal conductivity, density, softening point, elastic recovery and cone penetration. The simplicity of the preparation method along with environmental and economical advantages encourage using this modified composite material as an effective replacement in the mastic currently used.

Poster T3-17

Transylvania DIH - one stop shop for innovation

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Abstract. Transilvania DIH's mission is to address industry and societal challenges through innovation driven by digital technologies. We use cutting edge technologies like AI, HPC and Big Data to enable digital transformation processes, provide green/sustainable solutions that improve productivity, competitiveness, growth, and wellbeing at regional, national, EU, and international levels. Transilvania DIH's general objective is to provide a complete set of digital transformation and innovation services for (1) SMEs and (2) public sector organizations (PSOs) conducting non-economic activities from the NW region of Romania and, through the EDIH network, at EU level. TDIH's primary specialization and services use AI, HPC and Big Data to support the green and digital transformation of SMEs and PSOs in the fields of Digital Health and Industry 4.0, leading to economic development, competitiveness, and societal progress.

TDIH is based on a 3-phase process: Understand > Innovate > Scale, and 2 alternative Client Journeys (Minimal and Optimal) through which we will provide significant innovation and digital transformation services.

We will provide knowledge and technological transfer from research to the market by services: Testing/validation for software applied in energy; Testing components and equipment for energy efficiency and green buildings; Access to specialists; Training in the fields of energy transition and digitalization in energy.

Poster T3-18

Low voltage distribution harness cables

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Abstract. Low voltage distribution system is consisted of two parts - 1 Harness cable inside finger - 4 Harness cables inside girder for long barrel modules and 3 harness cables inside the girder for extended barrel module. These specifications refer to cable assemblies used for command and control of LVPS and distribution of low voltage to front end electronics inside Tile Calorimeter modules. Power Distribution in the Drawer New Brick Design: One +10V brick – Each brick has theoretically the same load current Each Mini Drawer half is powered by a single brick – One brick for each half Mini Drawer (4 Mini Drawers = 8 Bricks) – Point-to-point connections (prefabricated wiring) – Possibility of implementing redundancy (x2 current capability of bricks over nominal) Due to cable harness component materials (metal and plastics), only the Total Integrated Dose of ionizing radiation (TID) must be considered. ⎫ Based on radiation simulations of 4ab-1 of HL-LHC running by the ATLAS Radiation Estimation Task Force, the highest dosages encountered by harness cable components is inside finger: 80 Gy of TID of ionizing radiation. ⎫ The safety instructions IS23 for cables and IS41 for plastics and non-metallic materials must be complied.

Poster T3-19

Photopyroelectric technique: spectroscopic and calorimetric applications

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Abstract. An overall view of the development of the PPE technique is described, through which both theoretical and experimental aspects of PPE detection are explored. Several important examples of spectroscopic and calorimetric applications are also detailed. The applications section contains a selection of case studies that cover a wide variety of research fields. We show that the PPE technique is not only useful to investigate optical and thermal properties of various solids (homogeneous and porous, magnets, ferroelectrics, thermoelectrics, etc.) and liquids (binary and isotopic mixtures, volatile liquids, liquid foodstuffs, magnetic nanofluids), but simultaneously provides a good method to study physical processes (such as molecular associations or phase transitions).

Poster T3-20

Numerical modelling of integrated photocatalytic ozonation/ membranes filtration processes for water treatment

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Abstract. Water pollution represents the main way of aggression on the environment, because aqueous effluents act as an efficient vector in spreading chemical products. In order to avoid the impact of pollutants, new remediation processes and technologies was developed in recent years, technologies that must fulfill the role of removing target pollutants even in low concentrations in waste water or water sources. Advanced oxidation processes (AOP) are primarily intended for the quasi-total removal of hardly degradable organic pollutants or for their transformation into non-toxic and/or biodegradable secondary products, being suitable even for water volumes with a relatively low concentration of pollutants but with high negative impact. The innovative approach of a particular class of advanced oxidation processes (heterogeneous catalytic/photocatalytic ozonation) is proposed, integrated with membrane filtration processes in order to develop some POMR (Photocatalytic Ozonation Membrane Reactor) type reactors with applications in water treatment. The paper presents a theoretical approach and the development of a multiphysics numerical model using CFD (Computational Fluid Dynamics) concepts to establish the basis of conceptual design for a water decontamination unit.

Poster T3-21

Innovative Technologies of separating 6Li in order to obtain a separation factor as high as possible - A review

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Abstract. The purpose of this review is to establish a study on the innovative technologies of separation of 6Li in order to obtain a separation factor as high as possible, using safe materials for the environment and the operating personnel. The development of a 6Li enrichment technique in terms of technical reliability represents an important step in the worldwide fusion program. Fusion is the new solution for energy supply, and deuterium-tritium (D-T) reactors are the first generation of fusion reactors. One of the promising sources of tritium is obtained by bombarding lithium with neutrons.

Amalgamation has been investigated and applied in the past as a large-scale enrichment method. The COLEX (chemical exchange in columns) and ELEX (electrochemical exchange) processes were explored. The toxicity of mercury generated serious environmental problems for some reason the method was abandoned. To replace mercury, other compounds such as tin, gallium, zinc, graphite and metal oxides and sulfides were investigated. It was found that metals, metal sulfide and graphite preferentially take up 6Li, while metal oxides have a preference for 7Li. The enrichment factors related to these materials could not exceed those demonstrated by amalgamation.

Poster T3-22

Catalyst for oxygen and hydrogen recombination

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Abstract. In general, in any closed or open building housing where is an installation operating with hydrogen or in which an accumulation of hydrogen isotopes may occur, a method of rapid disposal must be provided to avoid ignition or explosion caused by reaching a concentration within inside the flammability/explosion limits. The presence and/or generation in the atmosphere of tritium isotope, nuclear facilities bring additional risks, caused both by its radiotoxicity but also by the risk of ignition induced by the presence of beta radiation. The need to remove or recover hydrogen isotopes by catalytic recombination with oxygen, from certain spaces and installations, occurs when it is not possible or not recommended to ventilate the internal atmosphere in the ventilation duct, especially when it is contaminated with tritium. That is why it is necessary to have a technology and an adequate, efficient and fast system to eliminate hydrogen and/or its isotopes, regardless of the concentration in which it is (from traces to stoichiometric mixture). A diverse range of hydrophilic catalysts have been developed and reported in the specialized literature generally based on noble metals, Pd or Pt/support, (Pt/Al_2O_3; Pt/SiO_2 Pt/TiO_2; metal oxides (CuO; NiO; MnO_2; Co_3O_4), Hopcalite I; Hopcalite II, etc. The paper proposes the evaluation of the currently existing catalysts, commercial or not, with a view to developing an own catalyst for the development of an efficient system for the recombination of hydrogen isotopes with oxygen.

Poster T3-23

The influence of cations on molybdate species distributions in molybdenum-copper-lead glass

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Abstract. Amorphous structures are ideal waste form candidates for High-level radioactive waste. PbO_2 is an unconventional network former, able to form an amorphous structure by creating three-dimensional spatial network with [PbO_4] and/or [PbO_3] structural units. Lead based glass has the potential to facilitate glass formation with a wide variety of radioactive wastes compounds very poorly soluble in conventional borosilicate glass. Also, lead is very good attenuator for gamma rays and, thus providing a radiation shield for nuclear waste. In this regard, we present the design and formulation of lead-based glass, as an alternative waste form to borosilicate glass considering to improve the solubility of Mo without phase separation in the presence of Cs^+ ions. X-ray diffraction, Fourier Transform Infrared, Ultraviolet-Visible and X-ray photoelectron spectroscopy were used to explore the physica-chemical properties and structural changes of molybdenum-copper-lead glass as a function of caesium oxide content. The obtained results are discussed in relation with defects formation, and cations influence on molybdate species distributions in lead-based glass.

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SECTION T4

Nanostructured and Hybrid Materials

Oral T4-1

Hemodynamic effects on particle targeting in the arterial bifurcation for a different type of functionalized magnetoresponsive particles

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Abstract. Inhibiting angiogenesis in atherosclerotic plaques and preventing restenosis in specific anatomical sites, such as arterial bifurcations, have been proposed as drug therapies for vascular disease. A combination of functionalized magnetic nanoparticles (MNPs) with external magnetic fields is particularly promising for enhancing the duration and local efficacy of medication release. In this study, we investigated the viability and effectiveness of the magnetic particle targeting idea at the artery bifurcation, which is the site of the lesion, utilizing a magnetic field generated by a locally placed external permanent magnet. In this publication, we studied the particle targeting efficiency for the Type D lesion (Type D: Stenosis involving the main vessel and ostium of the side branch), which is a result of the SYNTAX study (SYNergy between PCI with TAXUS™ and Cardiac Surgery). The primary objective of the studies is to investigate how the flow hemodynamics affects the rate of magnetic nanoparticle accumulation at the desired spot for various types of MNPs. The findings of the experiment demonstrate that different MNP types of deposit at various rates even when flow conditions are the same.

Oral T4-2

Design of mixed oxide nanostructured coatings on carbon backbones in composites used as a support for Pt electrocatalysts

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Abstract. The still unsurpassed properties of platinum supported on high surface area carbon make it the most widely used polymer electrolyte membrane fuel cells electrocatalyst. However, corrosion of the Pt/C catalysts results in continuous performance decrease and it is the limiting factor determining the life time of the cell. Our strategy is to combine the stabilizing effect of inorganic oxides (containing dopants as co-catalysts) with the good conductivity and high specific surface area of carbon materials in a unique composite system. We have demonstrated that by increasing the density of functional groups on carbon, it is possible to change the nucleation and growth of the rutile-TiO_2 phase, which has a positive effect on the formation of a nanostructured mixed oxide coating over the carbon. Structural, textural and morphological difference between the oxophilic metal (Mo, Sn)-doped TiO_2-carbon composites prepared using functionalized or unmodified carbon and the effect of carbon functionalization on the electrocatalytic behavior and stability of Pt catalysts will be demonstrated.

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Oral T4-3

CO_2 methanation on doped mesoporous silica structures

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Abstract. CO_2 emissions level at global scale has increased over the last years leading to global warming effect. As a result, measure have to be undertaken in order to reduce the carbon dioxide concentration in the atmosphere. One opportunity consists in transforming the CO_2 into valuable compounds like methane, methanol or higher alcohols. The methanation process is a catalytic reaction between CO_2 and H_2 gas in the presence of a metal-doped heterogeneous catalyst in order to produce synthetic methane. The heterogenous catalyst is of most importance due to its direct implication in the performance of the reaction. Mesoporous silica materials doped with metal/metal oxides can be used for the CO_2 methanation reaction due to their high surface area and ordered porous structure. Different methods of preparation have been performed in order to obtained a good dispersion of the metallic nanoparticles in the internal pores of the mesoporous silica support which may enhance the catalytic activity. The prepared catalysts were characterized by several physicochemical techniques (XRD, BET, H_2-TPR, and H_2-TPD). The catalytic performance of the synthetized mesostructured materials was investigated at ambient pressure in a temperature range of 150-500°C using Ni on mesoporous silica as catalysts and an online gas chromatography system to analyse the reaction products and calculate the CO_2 conversion and methane selectivity.

Oral T4-4

Ultra-small IONPs based phantom study for non-invasive MRI

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Abstract. Multi-modal imaging is one of the important characterization tools to explore in depth MRI for various biomedical applications. To perform the imaging analysis, excellent quality of small size nanoparticles are utilized to obtain 3D anatomical images. In view of this, ultra-small iron oxide nanoparticles (IONPs) and manganese-oxide based nanoparticles (Mn-Oxide), that exhibit a significant biocompatibility, magnetic properties, and morphology, are considered as potential candidates to replace Gadolinium-based contrast agents for non-invasive MRI application. Fabrication of both the types of nanoparticles poses an important challenge in obtaining a dispersion that meets physiological stability and relaxivity parameters (r_1 and r_2) for high resolution MRI. Our study focused on the synthesis of manganese oxide nanoparticles, nanocomposite of commercially obtained two-dimensional manganese oxide nanosheets (2D-MnO_2) and another nanocomposite of commercially obtained ultra-small IONPs with manganese oxide nanoparticles. Nanoscopic characterizations such as, Raman spectra, AFM, Ultra-centrifuge for purification, DLS, Zeta potential and UV-Vis spectra were performed to analyse synthesized material properties. THz spectroscopy was used to analyse chemical binding in the obtained complexes. A phantom-based MRI relaxivity study, was performed and a 3D-phantom images acquisition was planned.

Oral T4-5

Innovative Nanostructured Polymers Based on Renewable Resources for Heavy Metals Removal from Mining Wastewaters

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Abstract. Heavy metals contamination has significantly impacted the integrity and quality of all environmental factors worldwide. Researchers have made numerous attempts to develop new materials and to improve their capacity to remove this type of pollutants from wastewaters. We successfully prepared novel environmentally-friendly nanomaterials based on corn protein and applied them for heavy metals removal from mining wastewaters. The synthesized nanomaterials were characterized using a variety of analytical techniques, including transmission electron microscopy (TEM), dynamic light scattering (DLS), and Fourier-Transform infrared spectroscopy (FTIR), while the metal concentrations in solutions were determined via Atomic Absorption Spectroscopy (AAS). The adsorption processes were described using specific equilibrium isotherms and kinetic models. Significant changes in the physico-chemical parameters and 80% reduction on heavy metals content were obtained after using the nanostructured polymers. We conclude that zein nanomaterials can be recommended for further applications in the acid mine drainage treatment and remediation of mining areas.

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Oral T4-6

Interactions of Antimonene nanosheets with living cells: focus on the photodermal effect

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Abstract. Antimonene has gained considerable attention due to its unique properties and potential applications, though some aspects are still under investigation. It's strong light absorption and efficient photothermal conversion make it a promising candidate for photothermal activity. However, the precise mechanism of interaction between antimonene and human cells remains unclear, particularly at single cell level. In this study, antimonene nanosheets were successfully synthesized via liquid phase exfoliation in organic solvents, ensuring long term stability by incorporating a surfactant during synthesis. The synthesized antimonene was characterized using UV- visible Spectro photometry, Zeta potential and DLS measurements, RAMAN spectroscopy and Scanning emission microscopy (SEM) to elucidate its structural and functional properties. The research primarily focuses on exploring the biological applications of antimonene, particularly in photothermal activity. The aim is to understand its potential in photothermal therapy and expand its application in sensing. By shedding light on the interactions and behaviour of antimonene at the cellular level, this study aims to contribute the broader understanding of its applications, further investigations will uncover additional opportunities for antimonene in various fields, paving the way for its effective utilization in diverse applications.

Oral T4-7

Implementation of waste vegetable-derived carbon nano-platelets on laser-treated metallic electrodes for supercapacitors.

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Abstract. The increasing demand for renewable energy have required, in recent years, many efforts toward the development of energy storage devices. Due to their performances in terms of specific capacity, stored power density, reduced charge/discharge times, the different families of SCs are attracting attention of scientific community. Furthermore, they often show other advantageous aspects as cheapness, reduced environmental impact, long cycle life, and so on. For the performance of a supercapacitor, electrodes are undoubtedly crucial elements: here we present a brief overview on strategies and methodologies to improve performances of electrodes showing some possibilities of their optimization at the state of art. After presenting some results exploiting nanotechnologies and nanomaterials, or different approaches for the modification of metallic current collectors, the recent results concerning femtosecond laser-treated metal electrodes covered by graphene-like nanoplatelets obtained from waste vegetable mass will be shown.

Oral T4-8

Chemical growth of $GaFe_xO_y$ thin films – unravelling the effect induced by the processing parameters on the final stoichiometry

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Abstract. Chemical Solution Deposition (CSD) methods have been widely investigated for thin film growth for nearly three decades. The main advantages of the CSD method over physical deposition methods are: 1/ a good control over the chemical composition by changing the stoichiometric ratio of the starting materials; 2/relatively low processing temperature; 3/ it is cost effective. It is generally accepted that a range of requirements must be fulfilled by the solution chemistry, substrates, and processing conditions for successful implementation of this method. This work presents the growth of $GaFe_xO_y$ thin films on different single crystal substrates highlighting the influence of processing parameters on the final stoichiometry of the film. In this vein, the precursor solution concentration, the solvent chemical nature, the addition of additives will be considered. The rheological properties (viscosity, surface tension) and surface wettability (contact angle) of the precursor solutions will be discussed. Also, the thermogravimetric investigations of the precursor solutions will be done to tune the pyrolysis and crystallization processes in control atmosphere (air, O_2, N_2, Ar-5%H_2). The obtained films will be structural and morphological analysed via XRD, AFM, XRD techniques and the magnetic properties will be investigated, as well.

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Oral T4-9

Hybrid proton exchange membrane based on polysulfone and nanostructured silica

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Abstract. Commercial polysulfone was sulfonated with a mild sulfonating agent, trimethylsylil chlorosulfonate and then several amounts of mesoporous silica nanoparticles, between 5 and 15 wt %, was mixed in the sulfonated polysulfone solution, in dimethylacetamide. The membrane was recast from the solution, and the membrane samples were characterized by FTIR, SEM-EDX and thermal gravimetry. The proton conductivity of the hybrid membranes was determined by the electrochemical method and compared with the values of the state-of-the-art proton exchange membrane.

Oral T4-10

^{1}H NMR and complementary studies on cement based composites for additive manufacturing

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Abstract. A continuous effort is spent in the design and characterization of cement based composites for additive manufacturing. For such applications, the pastes must satisfy multiple requirements in terms of their pumpability, extrudability and buildability. We investigate the potential use of ^{1}H NMR relaxometry and complementary techniques, i.e. standard Vicat tests for setting time, extrusion tests, X-ray diffraction (XRD), ultrasonic pulse velocity measurements (UPV), microscopy and mechanical tests for paste characterization before and after hardening. White Portland cement is chosen as starting material, due to its low content in magnetic impurities and fast setting time. The effects of different parameters are investigated: (1) water to cement ratio (w/c) and the presence of (2) silica fume (SF), metakaolin (MK) (3) accelerator (A) and (4) superplasticizer (SP). The pozzolanic activity of SF and MK is evaluated from structural data, while good correlations were confirmed between the Vicat setting time and in-situ ^{1}H NMR studies on cement hydration, as well as between UPV and fracture strength of hardened samples.

Oral T4-11

Visible light photocatalytic activity of TiO_2/graphene-based composites

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Abstract. Ternary nanostructures of TiO2/graphene/metal nanoparticles were successfully synthesized via chemical and thermal treatment methods. We prepared a series of composites containing metal nanoparticles, reduced graphene oxide or nitrogen-doped graphene and titania nanotubes/nanoparticles for the degradation of model emerging pollutants (sulfamethoxazole, amoxicillin, acetaminophen or β-estradiol). The combination between the special characteristics of TiO2 (chemical stability, photocatalytic potential, increased electrical conductivity, non-toxicity) with the unique two-dimensional crystal structure of graphene (high specific surface area, excellent mechanical properties and electrical conductivity, thermal stability, good biocompatibility) leads to high efficiency photodegradation catalysts.

The surface morphology and structural aspects were assessed by SEM/TEM microscopy, powder X-Ray diffraction measurements and XPS spectroscopy, while the optical characteristics by measuring the DR UV-Vis spectra and calculating the bandgap energies. The alignment of the conduction (CB) and valence bands (VB) of the photocatalysts have been correlated with the reduction and oxidation potentials of the surface electrocatalytic reactions driven by the photogenerated e- and h+.

The photocatalytic performance was evaluated using a visible light source and the time evolution of degradation by high-performance liquid chromatography (HPLC). The influence of graphene or nitrogen-doped graphene in the composite is discussed in terms of its role in the mechanism of the photocatalytic process.

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Oral T4-12

Correlations at exceptional points in the spectra of non-Hermitian quantum systems

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Abstract. We investigate non-Hermitian PT-symmetric quantum systems that exhibit exceptional points in their spectra. These singularities mark a real-to-complex transition in the energy eigenvalues of the system and simultaneously the coalescence of two or more eigenvectors. It is shown that a system hosting such degeneracies displays spatial correlations that decay with anomalous power laws. Moreover, the entanglement entropy shows saturation above a correlation length, characteristic to an insulator, even though the spectrum is gapless. We demonstrate how such systems may be realized on gain and loss lattices, that might find a realization in photonics, acoustics, or various open quantum systems subjected to continuous monitoring.

Oral T4-13

Novel smart wound patch: the next generation of wound dressing

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Abstract. Appropriate treatment of wounds and skin infections has become nowadays extremely challenging, due to inefficient therapies and the rise of bacterial antibiotic resistance. With this in mind, we developed a novel smart wound patch with synergistic photothermal and antimicrobial properties to support efficient wound healing at the wound site. The exceptional properties of the as-developed smart patch are owed to the antimicrobial peptides (AMPs) and gold nanoparticles (AuNPs). First, spherical shaped AuNPs, synthesized using the seed-mediated growth procedure, employed herein as intrinsic photothermal-agents, were immobilized on round-shaped cotton patches *via* controlled dip coating and then integrated into a flexible PDMS substrate. The successful binding of three specific AMPs on the AuNPs surface was confirmed *via* UV-Vis and Raman spectroscopy. Moreover, three different irradiation sources, i.e. 532 nm laser, 530 nm LED and flashlight of a smartphone, were tested and compared in order to evaluate the effective response of the plasmonic patch. While the *in vitro* cytotoxicity assays confirmed indirectly the release of the AMPs from the wound patch under irradiation, the antimicrobial and antibiofilm properties were also evaluated. This state-of-the-art approach proves to be highly efficient, time-effective and low-cost, operating as a next generation of wound dressings with enhanced capabilities.

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Oral T4-14

Composite type of electrocatalyst supports for polymer electrolyte membrane fuel cells (PEMFCs) from novel carbonaceous materials

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Abstract. Polymer electrolyte membrane fuel cells (PEMFCs) convert chemical energy into electricity efficiently and environmentally friendly way. One of their main components is the electrocatalyst, most frequently carbon supported platinum. The stability of the carbon support often does not meet the requirements, which leads to a decrease in the activity of the Pt catalyst. Our approach is TiO_2-C composite supports, where TiO_2 provides higher stability than commercial carbon in acidic and oxidizing environments, the carbonaceous part contributes to the electrical conductivity. New types of carbonaceous materials, as derivatives of graphene, can also provide increased stability and conductivity. We prepared TiO_2-C composites from graphite oxide, multilayer graphene and their N-doped variations by sol-gel- and ball milling techniques. The primary consideration was to achieve the appropriate specific surface area (>100m^2/g). The morphology, surface properties and electrical conductivity were also investigated. The possibilities of the preparation of TiO_2-C supports by the different methods and the electrocatalytic behaviour of the Pt catalysts will be demonstrated.

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Oral T4-15

Hemisphere-void patterned gold electrodes for (EC-)SERS applications using colloidal template-directed electrodeposition

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Abstract. Electrochemical surface-enhanced Raman spectroscopy (EC-SERS) applications require nanostructured plasmonic electrodes. These electrodes should be mechanically and electrically stable, possess a uniform surface and allow a tuneable optical response. The aim of this work was to obtain hemisphere-void patterned gold electrodes by electrodeposition in the interstices of a polystyrene colloidal template, pre-assembled on top of a thin film gold working electrode surface. The plain electrodes were fabricated on Si by deposition of thin metal films of TiW / Au using magnetron sputtering with metal thickness in the range ca. 60-320 nm. Patterning in a three-electrode configuration was done by wet etching via a photoresist mask. The final dimensions of one chip were ca. 10 mm x 30 mm, and compatible with the standard connectors for spectroelectrochemical readout. The electrodeposited gold allows the subsequent removal of polystyrene spheres, creating therefore a large-area periodic array of gold hemisphere voids of few hundred nanometres diameter. The obtained periodical patterned gold electrode surface exhibits desirable optical and electrical properties, and therefore is a good candidate for EC-assisted SERS detection and analyses.

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Poster T4-1

Tumor apoptosis and cell cycle arrest induced by magnetic hyperthermia mediated by iron oxide nanoclusters

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Abstract. We synthesized iron oxide nanoclusters (MNC) stabilized with 3.4-dihydroxybenzhydrazide (DHBH) and then linked with doxorubicin. MNC morphology and elemental composition (TEM), surface chemical composition (XPS) and SAR measurements showed that the MNC were packed into clusters, with well-defined spherical shape and size ~ 200 nm, with high SAR value. The antitumor effects of magnetic hyperthermia (MH) mediated by the MNC against breast cancer cells *(*MDA-MB-231) was tested: cell toxicity (MTS assay), cellular uptake (TEM), apoptosis induction, cell cycle (flowcytometric analysis). Biological tests showed cell viability above the toxicity limit for concentrations of MNC w/wt doxorubicin up to 100 μg/ml. MH therapy mediated by MNC induced significant apoptosis, compared to control. Magnetic hyperthermia using MNC linked with doxorubicin, further increased cell death by apoptosis and necrosis and induced cell cycle arrest.

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Poster T4-2

Improved durability of styrene-isoprene-styrene triblock copolymer added with reduced graphene oxide

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Abstract. The duration of polymers is directly related to their oxidation strength. The prevention of polymer oxidation is offered by a large variety of antioxidants. The graphene/polymer composites may be a solution for an improved durability. This study addresses the obtaining of some long-term products, efficiently stabilized by reduced graphene oxide (rGO), with special applications such as electrical cable insulation, food packaging, sealing gaskets, etc. Styrene-isoprene-styrene triblock copolymer (SIS) improved with rGO may be used due to the functional properties available over an extended period of operation. The stability, efficiency, comparable price with other antioxidants recommended graphene as an antioxidant additive. The graphene oxide (GO) was synthesized from natural graphite powder by modified Hummer's method and reduced in the presence of ascorbic acid. rGO was added to SIS in concentrations of 1, 2 and 3 wt%. The samples were thermally treated in air at a constant temperature of 80°C for 5, 10, 15 and 20 h. The chemiluminescence procedure was used for the oxidation progress evaluation when the composite is oxidized at 130°C. The presence of graphene brings a significant slowing down of the oxidation rate. The graphene concentration increase leads to higher material stability extending the oxidation induction time.

Poster T4-3

Synthesis of a magnetic sorbent only from waste materials

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Abstract. The increasing pollution of the environment presents a large problem for today's society. Among different methods for the decontamination of water, adsorption attracts the most intensive research. Magnetic sorbents have the benefit of being easily removed by magnet and thus being able to subsequently be reused. Due to the large quantities of sorbents necessary, their preparation should be cheap and, if possible, using waste materials. However, most of the current research on this subject uses iron salts, which need to first be prepared using energy and hazardous chemicals, as precursor for the magnetic sorbents. We describe here a simple method using only iron mud, sawdust, and water to prepare the desired magnetic sorbents. Different materials were prepared by varying reaction conditions and the samples were analyzed by SEM, EDX, FTIR and magnetization measurements. Different dyes were then used as model pollutants to determine the optimum reaction conditions for preparing the magnetic sorbent.

Poster T4-4

The development of an ecosystem in Martian soil simulants

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Abstract. Three types of Mohave Mars Simulant (MMS) coarse, fine and superfine developed by NASA and JPL were analysed. These simulants represent the closest simulant to the actual Martian regolith. The characterizations of these Martian regolith were preformed using several advanced methods such as ^{1}H NMR relaxometry, FT-IR and near-IR VIS spectroscopy, as well as classical methods such as pH, electrical conductivity, total dissolved solids, turbidity, thermogravimetric measurements as well as optical imaging. The analyses showed that traces amounts of water nitrogen, phosphorus and potassium are present in the Martian regolith simulants. To demonstrate the fact that it is possible to live on Mars, a Martian Garden (Marsarium) was built with these three types of Martian soil, in which various vegetables have been planted. Then, two families of ants of 2 different species were introduced. The ants adapted to the imposed conditions, as they start to rearrange the environment by dug tunnels in the soils. The environmental conditions were systematically monitored using a series of air and soil sensors and microcontrollers.

Poster T4-5

Bio-polymer and hybrid nanocomposites: in vitro cytotoxicity against human cell lines

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Abstract. By creating new polymers through renewable resources, the environmental impact could be lessened and silicon-based nanoparticles are renowned for causing less cytotoxicity. In this study, we aimed to investigate the biocompatibility of Halloysite and Aerosil, which are two types of Si-based nanoparticles, used as precursors for bio-polymer nanocomposites. The nanoparticles were left to interact for 24 hours with normal (fibroblasts and keratinocytes) and cancerous (lung and skin) human cell lines. The cytotoxicity was assayed through biochemical methods (MTT and LDH), while the morphology was investigated through light microscopy. The results showed that Halloysite is affecting cells' viability more than Aerosil, except for A375 (skin melanoma), but without significant toxic effects. These fundamental findings show that the chosen precursors are suited for further analyses and investigations.

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Poster T4-6

Fabrication and SERS performances of hierarchical heterogeneous arrays decorated with star-like gold nanoparticles

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Abstract. Three dimensional (3D) surface-enhanced Raman scattering (SERS) platforms on solid or flexible substrates have exceeded the traditional sensing applications. The ease in achieving higher hot spots density in all three spatial directions is closely related to the fabrication versatility which combines modern *top-down* and *bottom-up* techniques. In this work, we developed an innovative 3D platform with advanced SERS capabilities by combining a wide range of fabrication techniques such as nanoimprint lithography (NIL), magnetron sputtering (MS) and chemical synthesis. Flexible, thermoplastic-based polymers have served as substrate to fabricate arrays of nanopillars using NIL and were metallized with plasmonic materials. Star-like gold nanoparticles (NPs) were further deposited on the nanopatterned surface to increase the abundance of the existing hot spots through the sharp spikes and dips, characteristic to this particular morphology. The contribution of the NPs to the overall signal amplification degree of test molecules (such as crystal violet, para-aminothiophenol) was assessed, while scanning electron microscopy (SEM) offered valuable information regarding the topography of the substrates.

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Poster T4-7

Graphene/TiO_2 nanotubes decorated with gold nanoparticles for efficient photocatalytic degradation process

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Abstract. The development of efficient photocatalytic materials for environmental remediation has become a critical research area due to the increasing demand for sustainable and clean technologies. In this study, we aim to present hybrid nanomaterials comprising graphene/TiO_2 nanotubes decorated with gold nanoparticles with enhanced photoresponse under visible light. The nanocomposites exhibit high photocatalytic efficiency towards the degradation of β-estradiol, excellent stability and reusability, making them promising candidates for various photocatalytic applications, including wastewater treatment and air purification. This study provides insights into the synthesis of advanced nanomaterials for sustainable environmental remediation, contributing to ongoing efforts to address the global challenges of reducing emerging environmental pollutants.

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Poster T4-8

Magnetic composite material for dental applications

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Abstract. The present research proposes the development of a new magnetic dental composite material, based on magnetic nanoparticle and/or magnetic clusters coated with a double layer of silicon dioxide, SiO2 and calcium hydroxide, Ca(OH)2 using a combined preparation method.

In general, this type of composite material finds its application in dentistry, in aesthetic restoration applications of dental structure, due to specific components of dental materials, which bring biocompatibility, chemical and mechanical stability but at the same time bring aesthetic improvements in terms of colour. In particular, each component of this dental composite material will bring particular benefits in specific dental applications.

An innovative property of this magnetic dental composite material is the presence of a magnetic phase in the composition, which allows to be applied to the tooth surface using an external magnetic field, which, compared to conventional application methods, has a major impact to reducing and smoothing the thickness of the adhesive layer, with a visible effect in minimizing the occurrence of dental caries under filling.

Poster T4-9

Surface-enhanced Raman scattering detection of endosulfan pesticide using colloidal nanoparticle architectures

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Abstract. Pesticides pose a great threat to human health and their rapid detection has become an urgent public safety issue, engaging the scientific community to search for fast and reliable detection techniques. Surface Enhanced Raman Spectroscopy (SERS) has emerged as a valuable detection tool due to its high sensitivity and selectivity, proving its suitability for the food industry and environmental monitoring applications. Endosulfan (ES) pesticide is a challenging analyte that has poor affinity to the metal surface and only few reports of SERS detection are presented in the scientific literature. Here, we present our various attempts for the SERS detection of ES using both colloidal suspensions and various types of nanostructured metallic films. The investigations showed that ES could be detected based on its SERS fingerprint down to 10^{-7} M concentration using silver colloidal nanoparticle suspensions. Aiming to limit the instability and unreliability of colloidal nanoparticles, nanostructured films were developed using techniques such as convective self-assembly, chemical assembly, and evaporation of metal films. SERS detection of ES using these substrates could be achieved by improving ES-to-metal surface interaction through chemical functionalization.

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Poster T4-10

Structural and optical properties of oxidic thin films fabricated by PLD

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Abstract. Pulsed Laser Deposition (PLD), as a physical deposition method, can be easily used for the fabrication of thin films of oxidic materials (in oxygen atmosphere, in order to replace the oxygen voids created by the plasma plume). The deposition conditions have been optimized for TiO_2 and Cu_2O thin films, followed by subsequent characterization (XRD; SEM; EDX and band-gap determination). These films are *n*-type semiconductors, and respective *p*-type semiconductors, and they are suitable for various classes of applications (photovoltaics, as thermoelectric elements, and so on).

Poster T4-11

MOFs supported NPs-catalysts for selective liquid-phase hydrogenation of nitrobenzene

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Abstract. Selective hydrogenation of nitrobenzene and its derivatives is one of the most important industrial reactions to produce their corresponding amines, which are versatile intermediates and precursors in the synthesis of organic compounds such as pharmaceuticals, pigments, dyes, polymers, and other fine chemicals. Currently, in the chemical industry the catalytic hydrogenation of nitrobenzene (NB) is the main process for the synthesis of aniline (AN) under various catalytic systems, in both vapor and liquid phase. About this process, the choice of catalysts, as well as the hydrogenation reaction conditions are the key factors to obtain high yield and superior selectivity for AN. Apart from other porous materials, the remarkable properties of MOFs provide clear advantages for application in heterogeneous catalysis. Recently, MOF-supported nanoparticles have been found to show excellent catalytic activity towards liquid-phase catalytic hydrogenation of nitrobenzene. In this study, we report the preparation, characterization, and the exploration of the catalytic performance of MOF-supported NPs catalysts: Pt/MIL-101(Cr) (2 wt.% Pt loading) and Au-Pt/MIL-101(Cr) (1 wt.% Au and 1 wt.% Pt loading) in the selective hydrogenation of nitrobenzene, under mild reaction conditions.

Poster T4-12

Crystalline Manganese Doped Copper Oxide Ability to Enhance Dopamine Electrochemical Detection

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Abstract. The hydrothermal approach was used to make undoped CuO and crystalline copper oxide that has been doped with manganese (CuO:Mn) at ambient temperature. Utilizing X-ray diffraction (XRD), transmission/scanning electron microscopy (TEM/SEM), and X-ray photoelectron spectroscopy (XPS), the materials were fully physico-chemically characterized. Furthermore, in electrochemical tests for a dopamine assay, their analytical usefulness was examined. The production of the CuO phase with good crystallinity was demonstrated by the XRD analysis, and the Mn doping was estimated by the XPS to be around 1 at.%. Square wave voltammetry (SWV) experiments using a screen-printed CuO:Mn modified electrode (CuO:Mn/SPE) at pH 5.0 under optimal conditions demonstrated a remarkable enhancement towards dopamine detection, with a linear response in the 0.1 - 1 M and 1 - 100 M linear ranges and a low limit of detection of 30.3 nM. Five times higher sensitivity for doped copper oxide material in comparison with un-doped sample was achieved A possible biomedical use for the created CuO:Mn/SPE electrode was also tested, with positive results on existing pharmaceutical medication.

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Poster T4-13

Magnetic sawdust used in oil adsorption

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Abstract. Considering the high pollution level in the environment, controlling and especially remediating pollutants has become a challenge. Oil pollution is one of the most important factors affecting the global environment and required the development of new materials and/or methods simple, with high adsorption capacity and environmentally friendly. The use of recyclable materials in the depollution process contributes to the global waste management system to support the circular economy. In our research we have proposed a method to recover oil from water using an innovative material based on sawdust impregnated with a hydrophobic magnetic composite material. Due to the porous structure of the sawdust and the magnetic properties of the as used composite material, the prepared absorbent system exhibited good absorption capacity and remote controllability. In addition, the proposed adsorbent system could also recover heavy underwater oil in the form of agglomerates that could later be separated from the oil/water mixture. This absorbent system has a huge potential to manage oil spills as well as organic solvent spills occurring accidentally in various industrial applications due to the easy availability of renewable sawdust, magnetic composite with very good hydrophobic properties and its easy production method and last but not least at very low cost.

Poster T4-14

MIL-53(Al)-derived Ni catalysts for CO_2 hydrogenation

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Abstract. Metal-organic frameworks' (MOFs) large surface area, tunable porous structure, ability to adsorb and store gaseous molecules, and their many other exceptional structural properties ensure an increasing use in the field of heterogeneous catalysis. MOFs are highly efficient in the hydrogenation of CO_2, as they can enhance the activation of the reagents used in the process. The special porous structure enhances the activation of carbon dioxide, while that of H_2 might be achieved by the increased metal dispersion provided due to the exceptional surface area. In this work, we report on the use of catalysts derived from the as-synthesized MIL-53(Al), impregnated with Ni nanoparticles, in the hydrogenation reaction of CO_2, all without a MOF activation process, thereby saving time and energy. The embedding of the 10 wt.% nickel loading into the structure of the MOF was carried out in two ways: by the classic wet impregnation method and by the melt infiltration method. In the case of both procedures, we investigated the influence of the impregnation temperature and time on the size, and dispersion of the nickel nanoparticles, and thereby on the catalytic performance in the CO_2 hydrogenation.

Poster T4-15

Evaluation of absorption and solubility of calcium phosphate cements in artificial saliva

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Abstract. Calcium phosphate cements are frequently used in biomedical applications due to their excellent properties such as bioactivity and biocompatibility. Different compositions can be used to formulate calcium phosphate cements. In the present work, three experimental cements composed of tricalcium phosphate, chitosan and hydroxyapatite were prepared. The aim of this study is to evaluate the absorption and solubility properties of these cements. The studies involved storing and weighing samples at different time intervals by immersing them in artificial saliva. Because the presence of artificial saliva temporarily moistens and lubricates the mouth, it is important to understand the effects of long-term use of this fluid on calcium phosphate cements. NMR relaxometry is used to investigate the absorption and solubility dynamics of samples. The results show that absorption of the investigated materials decreases with increasing immersion time and solubility is influenced by the type of organic matrix as well as the immersion liquid.

Poster T4-16

Dielectric properties of Layered Double Hydroxides (LDHs): a family of nanomaterials for Sensing, Energy and Environment

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Abstract. We focus on the dielectric properties of Layered Double Hydroxides (LDHs), two-dimensional ionic, lamellar and nanostructured materials, also known as hydrotalcite-like compounds or anionic clays. They consist of positively charged layers of divalent- or trivalent- cations, coordinated with hydroxyl groups. The global electrostatic neutrality is ensured by interchangeable anions intercalated between the layers with water molecules, which establish a network of hydrogen bonds providing additional active sites for external molecules. LDHs show a large specific surface area, high stability and permeability, biocompatibility, low cost, excellent workability, high compositional flexibility (tunable lamellar stoichiometry of cations and the choice of incorporated organic and inorganic anions), and anionic exchangeability. A great number of applications are reported in literature, ranging from biomedical fields (imaging for nanomedicine and drug delivery) to Energy Harvesting and Storage systems, from Sensing of organic and inorganic species to Metallurgy, from the field of Supercapacitors and Electrocatalysts to Environment applications such as water treatment systems. Moreover, several different applications arise from the post synthesis functionalization of LDHs nanoplatelets, or the choice of specific growth substrates (including flexible ones), their pre-treatment or suitable coating by metals. Some recent results and possible design of devices are reported.

Poster T4-17

Synthesis and characterization of MWCNTs decorated with Fe-doped ZnO nanoparticles for organic pollutant degradation

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Abstract. The present work reports the photoluminescence and photocatalytic properties of MWCNTs decorated with Fe-doped ZnO nanoparticles. MWCNT:ZnO-Fe samples with weight ratios of 1:3, 1:5 and 1:10 were prepared using a facile synthesis method. The obtained crystalline phases were evidenced by XRD. XPS revealed the presence of both Fe^{2+} and Fe^{3+} ions. EPR spectroscopy sustained the presence of Fe^{3+} ions and evidenced oxygen vacancies. TEM images showed the attachment and distribution of Fe doped ZnO nanoparticles along the MWCNTs with a star-like shape. All of the samples exhibited absorption in the UV region, and the absorption edge was shifted toward a higher wavelength after the addition of MWCNT. The PL emission spectra showed peaks in the UV and visible region. All of the samples showed photocatalytic activity against the Rhodamine B synthetic solution under UV irradiation. 96% degradation efficiency was obtained in case of MWCNT:ZnO-Fe(1:5) nanocomposite samples.

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Poster T4-18

Synthesis and characterization of W-doped TiO_2 nanoparticles for supercapacitors

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Abstract. In this work, W-doped TiO_2 nanoparticles were synthesized using the sol–gel method and were used as electrode materials in supercapacitor applications. The structural, morphological and compositional properties of the samples were analyzed by means of XRD, STEM, TEM, and XPS. The analysis of the defect centers was carried out using EPR spectroscopy. The electrochemical analysis of the assembled supercapacitor was done using cyclic voltammetry, galvanostatic cycling with potential limitation technique, potentiostatic electrochemical impedance spectroscopy, and voltage-holding experiments. All the presented samples showed paramagnetic defects in the EPR analysis, while 0.5% W-doped TiO_2 showed a maximum signal intensity. The equivalent series resistance (R_s) value for all the designs showed values under 1Ω. The supercapacitor performance of 0.5% W sample was tested with a newly designed five-electrode system with a specific capacitance of 25.5 F g^{-1} and with an energy density of 14.16 Wh kg^{-1} at 302 kW kg^{-1}.

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Poster T4-19

Eco-friendly synthesis of sulphur-doped graphenes with applicability in gallic acid electrochemical assay from food related samples

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Abstract. The emerging evidence over the past decade confirms that gallic acid (GA) plays a crucial role, with multiple pharmacological and therapeutic interventions in numerous health complications. Sulphur-doped graphene material (exf-SGR) was obtained from graphite rod electrochemical exfoliation in the presence of inorganic salts mixture $Na_2S_2O_3$ / $(NH_4)_2SO_4$ (0.2 M each), at low applied bias (6V). TEM/SEM images reveal the formation of large dimension graphene sheets having uniformly distributed spherical sulphur crystallites on the surface. XRD demonstrates that the material consists of few-layer S-doped graphenes. From XPS analysis the C/O ratio was determined to be 0.473 while C/S ratio equals 2.741, indicating a high heteroatom doping degree. Furthermore, the electrochemical performances of bare glassy carbon (GCE) and modified (exf-SGR/GCE) electrodes for GA assay were evaluated. The modified electrode shows a superior electrochemical behaviour over a broad GA detection range (0.1 – 100.0 μM), with a low detection limit (3.03×10^{-8} M). The electrode retains 96.83% of its initial response after 50 consecutive CV measurements indicating an excellent long-term stability and repeatability. The sensor possesses very good anti-interfering capabilities in complex matrix. The developed electrochemical sensor can provide a fast model for GA detection in food related and biological real sample analysis.

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Poster T4-20

Tunable and flexible 3D nanostructured surfaces with controlled architectures fabricated by nanoimprint lithography

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Abstract. The development of advanced materials and highly structured surfaces used in sensors for the detection of molecules and biomolecules is focused on two important approaches, "top-down" - which involves the miniaturization of devices by improving existing techniques and incorporating recent technological developments and "bottom-up" – which rely on stimulating atoms, molecules or nano-objects in order to organize and assemble into complex systems. Nanoimprint lithography (NIL) is a simple, reproducible, and scalable method to fabricate highly-ordered flexible three dimensional (3D) nanostructured surfaces over large areas. We report the fabrication of high-quality grating-type nanostructured surfaces with variable pitch using NIL technique which will serve as substrates in specialized sensors with improved properties for the detection of molecular analytes. To attain a precise replication of the mold into the substrate, we optimized the experimental parameters (the substrate temperature, pressure and imprinting time) in correlation with the chosen thermoplastic polymer (Zeonor, Topas, PMMA, polycarbonate, etc.). The topography for each imprinted polymeric substrate was evaluated using SEM technique.

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Poster T4-21

Kinetics for NO_2^- adsorption using an anion exchange resin, from aqueous solutions

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Abstract. The kinetic of NO_2^- adsorption onto Dowex-Marathon MSA anionic exchange resin, from different concentrations of aqueous solution was performed. To investigate the adsorption mechanism, four kinetic models were used: pseudo-first order, pseudo-second order, Elovich equation and intraparticle diffusion model, and the highest correlation factor (R^2) was obtained for pseudo-second order kinetic model. The concentrations of NO_2^- were performed using electrochemical measurements and the experimental data were interpreted with NOVA 1.11 software.

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Poster T4-22

Phonon-assisted tunneling current through a quantum dot coupled to a Majorana nanowire

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Abstract. We theoretically investigate phonon-assisted tunneling current through a quantum dot side coupled to a Majorana bound state hosted by the ends of a Majorana nanowire when the dot is connected to a single long-wave optical phonon mode. The behavior of the current-gate voltage, the current-bias voltage and the current-dot–Majorana coupling characteristics is analysed for an experimentally relevant parameter range. We find that the presence of Majorana zero modes leads to a suppression of the current when the gate voltage is pinned at the Fermi level, while an increase in the bias voltage counteracts this effect, in the absence of electron-phonon interaction. The effect of Majorana-dot coupling on the current-bias voltage characteristics alters depending on the bias voltage values in the presence of electron-phonon interaction. We also demonstrate that the current is most sensitive to, and non-trivially depends on the parameters of the Majorana circuit element at low temperature in low bias regime.

Poster T4-23

Rare-earth ions doping CeO_2 nanoparticles – insight into the correlation structure-morphology-photocatalytic activity

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Abstract. Cerium dioxide or ceria, CeO_2, is a n-type semiconductor with a band gap of 2.9 eV, which has been the subject of intense research over the last years due to its various applications, such as: solid oxide fuel cells as electrolytes, gas sensors, in catalysis/ photocatalysis, or in biomedical field for hyperthermia or as antibacterial agent, etc. The increasing interest in CeO_2 nanostructures in the photocatalysis comes from their reversible reduction-oxidation between Ce^{4+} and Ce^{3+} states, high oxygen storage capacity, and ionic mobility. These capabilities of ceria can be improved by suitable doping with various elements.

The present work presents the synthesis of rare-earth (Eu^{3+}, Gd^{3+}, Y^{3+}) doped ceria nanoparticles using a new facile and eco-friendly sol-gel method. This approach is based on the thermal decomposition of ceric ammonium nitrate, $Ce(NH_4)_2(NO_3)_6$ in the presence of a sucrose-pectin mixture. Therefore, our study is focused on a detailed structural, morphological, and optical characterization of the samples using X-ray diffractometry (XRD), UV-Vis, Raman and IR spectroscopies, high-resolution transmission electron microscopy (HRTEM), electron paramagnetic resonance (EPR) and photoluminescence spectroscopy (PL). All above mentioned are correlated to improve the understanding of the photocatalytic mechanisms involved in the degradation of organic pollutants by rare-earth doped ceria-based compounds and how the doping modifies the photocatalytic response.

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Poster T4-24

Structural and dynamic characterization by ^{1}H NMR and FTIR analyses of oils obtained from waste plastics by low temperature slow pyrolysis

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Abstract. The present study deals with converting waste packaging plastic materials - high density polyethylene (HDPE), polypropylene (PP) and polystyrene (PS) - in their combustible condensates, by slow pyrolysis at low temperatures, using an in-house made reactor inspired by the Blest machine model. In order to perform their structural characterization, the plastic materials, their respective pyrolysis products, and three liquid fossil fuels were analysed by advanced ^{1}H relaxometry and double quanta nuclear magnetic resonance (NMR) measurements, as well as Fourier transform infrared (FTIR) analysis. The condensate oils obtained by the thermal decomposition of plastics were collected unfiltered. Their calorific characteristics were determined and compared with those obtained for the conventional liquid fossil fuels.

Poster T4-25

Thermal conductivity enrichment for a novel thermoplastic polymer by using different filler

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Abstract. Achieving high heat conductivity of polymer composites employed in electronic devices is crucial, on one side and developing new polymers and polymeric composites with fluorine atoms has recently generated much attention, on the other side. The reason for choosing fluorinated polymers is made due to their excellent dielectric characteristics, low surface energy, strong hydrophobicity, low water absorption, and excellent chemical resistance. This work illustrates the synthesis, characterization, and discussion regarding the thermal management of a new fluorinated aromatic polyester and its composites. Poly(fluoromandelic acid) (PFMA) is a new polymer with multiple fluorine atoms on the polymer chain. The structure of the resulting PFMA consists mainly of a polyester backbone decorated with p-fluorophenyl groups and has carboxyl and hydroxyl groups at the ends of the polymer chain. Mass spectrometry, solid-state ^{13}C nuclear magnetic resonance, liquid NMR, FTIR, and Raman spectroscopy elucidated the polymer chain structure. The polymer composites were structural and morphologically investigated by FTIR spectroscopy and SEM microscopy. Thermal conductivities and diffusivity of PFMA and its composites were measured by the transient plane source technique, also called the Hot Disk method.

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Poster T4-26

Wheat straws as raw material for biogenic silica

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Abstract. Wheat is one of the most planted food crops in the world. Wheat straw are by-products generated in large quantities every year. Beside animal feed or fertilizer, wheat straws are used as fuels for heat or additives in building materials, causing significant environmental issues. More recently, wheat straw has been applied as the raw material for silica obtaining, in order to produce porous silica with low cost and high efficiency. In this study, the wheat straws potential as raw material for biogenic silica extracting was investigated. High-purity biogenic silica (more than 94 wt.% SiO_2) was obtained from agriculture wastes (wheat straw). Two different morphological forms of biogenic silica were obtained. The wheat straws were cut in small pieces and soaked in ultrapure water for 24 h, in order to swell the cell walls. The wet biomass was leached using 5 M sulfuric acid and 5% citric acid for a defined period, then calcined at 550 °C. The final products were characterized by XRF, FTIR, TG analysis, specific surface, pores distribution, and SEM. The obtained silica presented a microstructure composed of accessible, interconnected, and intra-particle mesopores (around 3.7-5 nm pores diameter) and high specific surface are (around 150 m^2/g).

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Poster T4-27

The impact assessment of multiwall carbon nanotubes functionalized with metal oxides on *Lactuca sativa* L.

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Abstract. This work aimed to assess the impact of several nanomaterials (CNT-COOH, CNT-MnO_2, CNT-Fe_3O_4, CNT-MnO_2-Fe_3O_4, MnO_2, and Fe_3O_4) on lettuce (*Lactuca sativa* L.). The plants treated with nanomaterials and the control plants (untreated) were grown in a growth chamber, in controlled conditions of light, temperature, and humidity. The results obtained indicated that depending on the nanomaterials used for the treatments, the content of bioactive compounds and the antioxidant capacity varied in comparison with the control plants. The treatments with CNTs functionalized with metal oxides conducted to an increase in the elemental content of the *L. sativa* leaves. Generally, the treatments with metal oxide nanoparticles and carbon nanotubes functionalized with carboxyl groups induced a decrease in the elemental content. The largest number of elements was affected by soil amendment with MnO_2 nanoparticles. In conclusion, the effect of carbon nanotubes decorated with Fe and Mn oxides have both a positive and a negative effect on the biochemical qualities of lettuce plants.

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Poster T4-28

Charge/spin transfer at interfaces between thin ferromagnetic films an 2D semiconductors

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Abstract. Composite materials with tailored properties can be engineered through combined dimensionality and proximity effects. Magnetic proximity effects refer to the phenomenon where a magnetic material can influence the magnetic properties of an adjacent non-magnetic material. Due to their potential applications in spintronic half-metals interfaced with 2D materials are of interest. In the present work the FePt (L10) half-metal films are covered with either ZnS, MoS2 or graphene layers through pulsed laser deposition (PLD). Here, through a double exchange mechanism, the semiconductor becomes ferromagnetic and couples with the half-metal. The process is driven by the energy bands setup at the interface. The FePt thin films on Al_2O_3 substrates were deposited by PLD in vacuum at 700 0C. Then series of either ZnS, MoS2 or graphene of various thicknesses were prepared onto FePt/ Al_2O_3 thin films. XRD, photoelectron spectroscopies, and electronic microscopy were used to characterize structures, composition and morphology of samples. Their specific properties were determined by using magnetometry, spin/charge transport and optical absorption and discussed in terms of spin polarized charge transfer.

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Poster T4-29

Particularities of polydopamine analogues

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Abstract. Polydopamine and its analogues belong to poly-catecholamines, a versatile class of polymers with applications in many domains like biomedicine, catalysis, water treatment, sensors, energy storage, etc. Adjusting the chemical structure of the starting monomer by modification of aromatic ring, substitution of the alkyl chain with different functional groups you could improve a specific application that you required. In the present work we focus in the design of new monomers substituted with different functionalities on the alkyl chain and their polymerization mechanism with specific proprieties. Each of these new polymers provide a unique mechanism in bulk or as coating, from fluorescence, hydrophilicity, surface morphology, thickness, antibacterial activity, cytotoxicity and so on.

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Poster T4-30

Synthesis and structural characterization of modified mica surface used as pollutant removal

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Abstract. Mica is a group of phyllosilicate minerals that includes minerals with almost perfect basal cleavage. Sheet of mica are used as insulating parts of electrical equipments. It is also used in paints, automotive plastic production, cosmetics etc. As an easily available naturally occurring material, due to its specific surface properties (surface charge, physical and chemical stability etc.), mica could be a good candidate as adsorbent for different pollutants (heavy metals, pesticides, pharmaceutical products, food dyes). In this study, the synthesis and characterization of mica based adsorbents functionalized with metal oxides were performed. For surface modification iron and copper oxides were used in different combinations. The structural and morphological characterization was carried out using, among others, X-ray diffraction, Brunauer-Emmett-Teller, Fourier-transform infrared spectroscopy methods.

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Poster T4-31

Enhanced Acetaminophen Electrochemical Sensing Based on Nitrogen-Doped Graphene

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Abstract. Due to the widespread usage of acetaminophen and the danger of harmful overdosing effects, developing appropriate procedures for its quantitative and qualitative assay has always been an intriguing and fascinating problem. A quick, inexpensive, and environmental friendly approach based on d.c. anodic graphite rod exfoliation in the presence of inorganic salt aqueous solution (0.3 M $(NH_4)_2SO_4$) has been established for the preparation of nitrogen-doped graphene (exf-NGr). The XRD analysis shows that the working material is a mixture of few (76.43%) and multi-layers (23.57%) of N-doped graphenes. From XPS, the C/O ratio was calculated to be 0.39, indicating a significant number of structural defects and the existence of multiple oxygen-containing groups at the surface of graphene sheets caused by heteroatom doping. Furthermore, the electrochemical performances of glassy carbon electrodes (GCEs) modified with exf-NGr for acetaminophen (AMP) detection and quantification have been assessed. The exf-NGr/GCE-modified electrode shows excellent reproducibility, stability, and anti-interfering characteristics with improved electrocatalytic activity over a wide detection range (0.1–100 μM), with a low limit for AMP detection (LOD = 3.03 nM). In addition, the developed sensor was successfully applied in real sample analysis for the AMP quantification from different commercially available pharmaceutical formulations.

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Poster T4-32

Add-on sensors for photovoltaic panels

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Abstract. Photovoltaic (PV) panels convert solar energy into electrical energy and the conversion process is negatively influenced by the rise of the temperature of the panel. This poster presents the concept of an add-on sensory platform that can be attached on commercially available (photovoltaic) PV panels. The sensory platform is meant to collect and transmit data from on-board sensors, from the temperature sensor attached on the non-irradiated (back) side of the PV panel and from an energy measurement module. Hence, the platform measures the energy drawn from the PV panel, the temperature of the panel and the intensity of the incident light. The sensory platform is able to store locally acquired data. A wireless module, contained by the platform, enables the platform to send data through LoRa communication.

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Poster T4-33

Facile preparation of PVDF / $CoFe_2O_4$-ZnO hybrid membranes for water depollution

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Abstract. The aim of this work was to fabricate a low-cost hybrid membrane with self-cleaning capability under visible irradiation and good stability applied for organic pollutant removal from waters. PVDF membrane modified with $CoFe_2O_4$-ZnO nanocomposites was prepared by phase inversion method in the presence of a magnetic field. The structural and morphological modifications induced by the presence of $CoFe_2O_4$ -ZnO nanocomposites were studied by XRD, FT-IR and SEM. The presence of $CoFe_2O_4$-ZnO nanocomposites increases the hydrophilic character of the membrane enhancing the antifouling capacity of the PVDF membrane. The influence of the $CoFe_2O_4$-ZnO amount on the photocatalytic activity of the membrane was studied by following the RhB degradation under visible light irradiation. Scavengers test coupled with EPR spin trapping technique allowed to identify the reactive species involved in the photocatalysis and to elaborate a pollutant degradation mechanism.

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Poster T4-34

Highly Sensitive Graphene-Based Electrochemical Sensor for Nitrite Assay in Waters

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Abstract. The growing use of nitrogen fertilizers and additives containing nitrite in food has increased exposure and, as a result, generated concerns about the harmful health consequences. This work presents the development of an electrochemical sensor based on graphene/glassy carbon electrode (EGr/GC) with applicability in trace level detection of nitrite in water samples. From the structural characterization of the exfoliated material, graphene sample appears as a mixture of graphene oxide (GO; 21.53%), few-layers graphene (FLG; 73.25%) and multi-layers graphene (MLG; 5.22%) and exhibits remarkable enhanced response towards nitrite compared to the bare electrode (three orders of magnitude higher). The EGr/GC sensor demonstrated a linear range between 3×10^{-7} and 10^{-3} M nitrite for square wave voltammetry (SWV) and between 3×10^{-7} and 4×10^{-4} M for amperometry (AMP), with a low limit of detection LOD (9.9×10^{-8} M). The practical applicability of the sensor was tested in commercially available waters with excellent results.

Acknowledgements. This work was supported by grants from the Ministry of Research, Innovation and Digitization, CNCS/CCCDI—UEFISCDI, projects number PN-III-P2-2.1-PED-2019-2410 (500PED/2021), and PN-III-P1-1.1-TE-2021-0358, and through the 'Nucleu' Program within the National Plan for Research, Development, and Innovation 2022–2027, project number project PN 23 24 03 01.

Poster T4-35

Electrochemical Sensor for the Quality Control of Novel Doxorubicin Pharmaceutical Formulations

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Abstract. Doxorubicin (DOX) is a chemotherapeutic agent used in the treatment of various cancers. Like other chemotherapeutics, DOX presents cytotoxic activity on both malignant and healthy cells, leading to adverse events. To reduce these adverse events, DOX can be encapsulated in drug delivery systems that deliver it selectively to the tumour. In the development of these pharmaceutical formulations, it is important to quantify the amount of DOX that is encapsulated and released from these carriers. In this work, an electrochemical sensor for the detection of DOX was build using in-house screen-printed electrodes. The surface of the electrodes was modified with gold nanostructures which improved their conductivity, improving the sensitivity towards DOX. The electrochemical behaviour of DOX was investigated, and the detection conditions were optimised. A calibration curve was built and a limit of detection of 0.33 μg/mL was obtained. A second aim of this work was the development of nanosome-based pharmaceutical formulations for the delivery of DOX. The amount of DOX released from the nanosomes was measured using both the electrochemical method and UV-Vis spectrophotometry, with good correlations between the two methods. This indicates the feasibility of using electrochemical methods for the quality control of pharmaceutical formulations containing DOX.

Acknowledgements. A.P. acknowledges UMF internal grant no 773/9/11.01.2023

Poster T4-36

Development of composite – cement materials: XRD, FTIR and NMR study

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Abstract. The cement manufacture is the third largest industry in the terms of energy consumers and generates approximately 7 % of the total CO_2 emissions in the atmosphere. The use of supplementary materials such as limestone, $CaCO_3$ and finely divided silica as a replacement of Portland cement was studied in the last years because serves to reduce CO_2 emissions and to save energy and natural resources. By addition of limestone to the clinker a significantly reduce of CO_2 emissions was reported. Finely divided silica fume can accelerated the hydration of cement in the concrete. In this paper, the effect of substitution of the limestone - silicate composites in the validated and expired cement material was investigated by X-ray diffraction (XRD) data, Fourier Transform InfraRed (FTIR) and Nuclear Magnetic Resonance (^{1}H NMR) relaxometry spectra. The composite materials were prepared by wet chemical method using as precursors broken (window) glassy powder and the recycled powder from construction and demolition waste.

Acknowledgments. This paper was supported by the Romania - Polish Academy project.

Poster T4-37

One-pot synthesis of Au/TiO_2±graphene oxide photoactive nanocomposites

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Abstract. Gold-TiO_2±graphene oxide nanocomposites were synthesized through a facile one-step hydrothermal method, followed by heat treatment at 700°C in oxygen-free atmospheres (Ar and Ar/H_2). The prepared nanocomposites were investigated in terms of structural (X-ray diffraction, XRD), morphological (scanning electron microscopy, SEM) and optical (UV–visible spectroscopy, UV-Vis) properties. XRD analysis revealed the presence of TiO_2 crystalline phases (anatase and rutile) as well as gold nanoparticles. SEM images showed that Au nanoparticles were loaded on the surface of both TiO_2 nanotubes and graphene oxide sheets. The study on the optical properties of the nanocomposites showed a red shift towards visible light region for Au/TiO_2 and Au/TiO_2-graphene oxide, indicating the bandgap narrowing of these samples. By extending their photoactivity to the visible light region, the prepared nanocomposites enable the efficient use of sunlight in the photocatalytic degradation processes of organic pollutants from water.

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Poster T4-38

Biochar applied for tartrazine adsorption

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Abstract. Biochar is a carbon-rich product resulting from the thermochemical conversion of carbonaceous materials in an oxygen-deficient environment at temperatures above 350°C. Biochar's multi-functional nature enables additional application scenarios beyond its conventional use as a carbon sink in soil, ranging from water filtration, and sensing application to its use as a building material, while largely retaining most of its carbon sequestration potential. In the last few years, the use of biochar as an attractive adsorbent material for the removal of several chemical and biological contaminants increase. This is due to its large surface area, porosity, and presence of various surface functionalities. The tartrazine is one of the most commonly dye used in a variety of food products as a coloring agent with potential health impacts. Thus, it is very important to determine and remove it from food products and waters. The scientific community has developed different decontamination protocols (e.g., adsorption, coagulation, flocculation, ozonation, photocatalysis) to reduce negative impacts on the environment. The aim of this study was focused on the characterization and application of biochar for removal of tartrazine from aqueous solutions. In order to establish the conditions for the optimal retention of tartrazine, the influence of some physico-chemical parameters on the adsorption process were evaluated. Among the examined parameters were the following: the initial pH, temperature, adsorbent dose, contact time, as well as the initial concentration of the dye solution. The best results were obtained to pH 2 and 30°C for 0.9 mg/mL adsorbent dose.

Acknowledgments. This work was supported through the Core Program within the National Research Development and Innovation Plan 2022-2027, carried out with the support of MCID, project no. 27N / 03.01.2023, component project code PN 23 24 01 03.

Poster T4-39

Chemical synthesis of Al_2O_3 particles from aluminum beverage cans

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Abstract. Recycling metal products is an economically and environmentally feasible way for obtaining and using metals as it requires less energy than needed for metal production. Due to their lightweight material, durability and higher recycling rate, aluminum beverage cans are considered one of the most versatile and popular beverage packages. In this work, Al_2O_3 particles were obtained from aluminum cans by chemical precipitation and calcination method. The produced metal oxide powders were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), electron paramagnetic resonance (EPR), and Brunauer-Emmett-Teller (BET) method. Prepared alumina powders would be suitable for several applications, including catalyst supports.

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Poster T4-40

ZnO based photocatalysts recycled from spent alkaline batteries

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Abstract. Due to its essential involvement in many applications, ZnO, a common semiconductor fulfills the requirements of multifunctional material. ZnO is used across multiple industries such as electronic, pharmaceuticals, agriculture, environmental and food. The growing use of ZnO resides from their intrinsic properties which make them amongst the most materials suitable in as mentioned industrial sectors. In the last decade, a large number of electrical and electronic wastes were released in the environment due to the rapid technological development, as well as digitalization. Recycling of ZnO from electronic wastes (E-wastes) is a key technology for sustainability maintaining and developing our society from viewpoints of energy and environmental issues.

In the present work, we focus on the recycling of ZnO-based nanostructures from spent alkaline batteries, further these being used as stable photocatalysts for the degradation of organic compounds in waste surface waters.

ZnO-based nanostructures were obtained from spent batteries using mild hydrometallurgical method, annealed at different temperatures and further characterized to prove their properties. Thus, the samples were characterized by XRD, TEM, FTIR, UV-VIS, PL and TGA. Photocatalytic tests evidenced that the recycled ZnO nanostructures show photocatalytic activity toward degradation of RhB dye and OTC. These approaches open a new way to circular and sustainable economy.

Poster T4-41

Hydrogel with graphene for drug delivery

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Abstract. The aim of the present work is the synthesis and characterization of a hydrogel drug-delivery system. The hydrogels are often chosen for these systems due to their unique physical-chemical properties that can guarantee a good drug release over time. However, the release from these structures is mostly driven by pure diffusion and to overcome this limitation the hydrogel can be "enhanced" with nanoscale fillers such as graphene. Therefore, the system developed, is made of three principal elements: biopolymer, graphene and drug. The synthesis of the graphene-laden hydrogels was carried out from the mixture of two solutions, one of polyacrylic acid and agarose and the other with graphene that was earlier prepared through the exfoliation method assisted by microwave irradiation. The system was then characterized by FTIR and it showed the characteristic vibrational bands of polyacrylic acid, agarose and graphene. Cytotoxicity tests were carried out on the samples showing that the overall viability of cells was not affected. The drug-delivery system was obtained adding dopamine to this hydrogel. Release tests were carried out at 25°C, 37°C and 44°C for 77 hours , the release was studied in 2 media: PBS (phosphate buffer solution) (pH 7.4) and bidistilled water. The presence of dopamine was then confirmed through UV spectroscopy. The UV analysis showed that dopamine is not stable enough to be measured in water, instead of PBS. The release profile showed the dopamine in the first fifth hours of sampling and after that dopamine started to auto-oxidate.

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Poster T4-42

Preparation of Al modified TiO_2 materials to promote photocatalytic activity

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Abstract. A mixed precursor containing aluminium recovered from end – of – life vehicles and TiO_2 Degussa P25 was used to prepare TiO_2 modified Al photocatalyst through solid state reaction. Al waste and TiO_2 Degussa P25 in the ration of n(Ti) / n(Al) = x (x = 0.0; 0.5; 1.0; 1.5; 2.0 and 2.5, note as 0.0, 0.5, 1.0, 1., 2.0 and 2.5% Al), and acetylacetonate and Tween 80 was mixed under magnetic stirring and sintered using a conventional furnance at 500°C. The thermal, structural, optical properties and photocatalytic activity for those as-prepared samples are demonstrated by: DTA – TG – DTG, X – ray diffraction, Fourier – transform infrared and UV – Vis spectroscopy. The effect of aluminium concentration on the characteristics of TiO_2 Degussa P25 depending on the above instruments are studied. The results revealed that the materials have crystal structure of anatase TiO_2, rutile TiO_2 and aluminium. The opto-electronic properties shows that Al addition shifted the absorption spectra toward the visible range. The photocatalytic performance of Al – TiO_2 composites was quantified by the degradation of Allura Red solution under a visible condition.

Poster T4-43

Solvatochromism effect in new polydopamine analogues

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Abstract. The chemistry of polydopamine analogues has received special attention in recent years due to the maintenance of adhesion properties to multiple surfaces by keeping the classic polymerization conditions, but also by modifying various properties such as biocompatibility, antibacterial, photocatalysis or optics. In the present case, by manipulating the structure of the monomers, by substituting the alkyl chain with amino groups, we studied their optical behavior for both the monomer and the polymer. One of the main properties of the new polymers compared to the controversial polydopamine is solubility. The choice of solvents influences both the intensity of the signal and the displacements obtained both in UV-Vis and in fluorescence. In the case of the new polymer, which is more precisely a complex assembly of different oligomers, a preferential behavior for certain solvents can be observed. Based on the results obtained in UV-Vis and fluorescence we can conclude the influence of functional groups in the formation mechanism of the new polymer and their introduction into the class of fluorescent polymers.

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Poster T4-44

PVDF membranes modified with Ni-Co ferrites for water treatment

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Abstract. Photocatalysis technology is an effective method for the removal of organic pollutants from water. The catalyst loss in separation process from suspension system represents an important drawback of photocatalytic technology. This issue could be solved by immobilization of catalyst on porous materials like activated carbon and membranes. Membrane filtration technology can efficiently separate suspended solids, bacteria and macromolecule solutes. By combining photocatalysis and membrane filtration technology the efficiency for pollutants treatment can be enhance due to a series of synergistic effects which appears. Based on the above mentioned, in this study were synthesized and Ni-Co ferrites nanoparticles. The synthesized nanoparticles were used to modify the polyvinylidene fluoride (PVDF) for obtaining ultrafiltration membrane with photocatalytic activity under visible irradiation. The synthesized Ni-Co ferrites were characterized by X-ray diffraction, and spectroscopic techniques. Also, the influence of Ni-Co ferrites on morphology, and hydrophilicity of PVDF membranes was studied. Rhodamine B dye solution was used as model pollutant to evaluate photocatalytic activity. The photocatalytic mechanism was elucidated based on the identification of radical species generated by the sample and in accordance with energy bands alignment. The presence of radical species at the solid–liquid interface was evidenced using ESR experiment coupled with spin-trapping technique.

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Poster T4-45

Photodegradation of acetaminophen and ibuprofen mediated by visible-light and Ni-TiO_2 nanotubes catalysts

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Abstract. Acetaminophen (paracetamol) and isobutylphenylpropionic acid (ibuprofen) are widely used drugs for controlling different medical conditions on human body, as such causing contamination of the aquatic environment. One of their remediation techniques is photodegradation. We prepared a series of composites containing NiO-titania nanotubes-reduced graphene oxide (20 wt%) or nitrogen-doped graphene. The surface morphology and structural aspects were evaluated by SEM/TEM microscopy, X-ray powder diffraction measurements and XPS spectroscopy, while the optical characteristics by measuring the DR UV-Vis spectra. Changes in the photodegradation efficiency of ibuprofen were observed when the hydroxyl radical production was carried out using H_2O_2 in the process. In general, photodegradation is more efficient in the presence of thermally reduced graphene oxide over nitrogen-doped graphene, demonstrating the influence of graphene in the composite.

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Poster T4-46

CoNPs electrodeposition on screen printed electrodes for cymoxanil detection

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Abstract. Metal nanoparticles (NPs) are widespread used in various scientific fields including biochemistry, optics, heterogeneous catalysis and plasmonic, but also employed in electrocatalysis. In this work cobalt nanoparticles (CoNPs)/ modified electrode was prepared by electrodeposition of CoNPs on the screen-printed carbon (SPC) electrode, which was characterized by scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS). It was found that a large amount of CoNPs with diameter between 120 nm and 230 nm was grown on the surface of SPC. CoNPs were applied to construct an enzyme-free sensor CoNPs/ SPC for cymoxanil detection in PBS solution pH 6, with an electrochemical efficiency of 123% compared to the unmodified electrode.

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Poster T4-47

Synthesis and characterization of $CoFe_2O_4$ magnetic nanoparticles and $CoFe_2O_4$-$BaTiO_3$ magnetoelectric core-shell nanoparticles

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Abstract. Magnetoelectric nanoparticles are widely researched due to their ability to control an electric field in structures at the nanometer scale, using an external magnetic field. Cobalt ferrite nanoparticles (CFO) were synthesized using a solvothermal method. The BTO was deposed on the CFO core particles using a sol-gel method to form $CoFe_2O_4$-$BaTiO_3$ (CFO@BTO) magnetoelectric core-shell nanoparticles. X-Ray diffraction shows single-phase CFO and BTO structures. Transmission electron microscopy reveals the core-shell morphology and an appropriate size for possible biomedical applications. Magnetic measurements were performed using a VSM. The hysteresis curves show a combination of ferrimagnetic and superparamagnetic behaviour for the cobalt ferrite cores.

Poster T4-48

Peptide dopped ORMOSIL nanoparticles: preparation, characterization and efficiency testing on human cancer cell lines

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Abstract. The In this study two types of ORMOSIL nanoparticles were obtained, difference between them being the substance used for precipitating the nanoparticles. Each type of nanoparticles was dopped with Gramicidin A peptide. Nanoparticles, simple or peptide dopped, were characterized using DLS, UV-VIS and fluorescence spectroscopy and SEM microscopy. When ammonia is used for precipitating the nanoparticles, the average size of them is 36.6 nm, compared to 41.6 nm, which is the average size of nanoparticles precipitated with APTES. These dimensions were obtained from DLS measurements, and confirmed by SEM. When Gramicidin A is used as doping agent the average sizes of nanoparticles increase to 60.6 nm, for nanoparticles precipitated with APTES, and 119.6 nm in case of precipitation with ammonia. The coupling between Gramicidin A and nanoparticles was probed using fluorescence spectroscopy, in comparison with Gramicidin A dissolved in the same buffer as nanoparticles. The efficiency of nanoparticles, simple or dopped with Gramicidin A, was tested against one healthy and three cancer human cell lines.

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Poster T4-49

New flexible wound dressing with antimicrobial capabilities using PDMS functionalized with AuBPs-AMPs complexes

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Abstract. During this era, in which antibiotic resistance of pathogenic bacteria represents a serious challenge, the research for new, more effective, easy-to-use, and low-cost alternatives to classical wound treatment has become essential. Due to their properties and increased affinity for bacteria, antimicrobial peptides (AMPs) have draw attention and are seen as "a new hope" in the biomedical field. This study focused on preparing flexible wound dressing with antimicrobial capabilities using PDMS coated with gold nano-bipyramid (AuBPs), which show advantages for both biosensing and therapy applications, further functionalized with AMPs. Several known AMPs were investigated against two bacterial strains: *Escherichia coli (*ATCC 8739), a model microorganism for *Gram-negative* bacteria, and *Staphylococcus aureus* (ATCC 6538), a model microorganism for *Gram-positive* bacteria. The new wound dressing was characterized by UV-Vis, thermal analysis, AFM, and SEM. The substrate biocompatibility was investigated against skin cells. The preliminary *in vitro* results point out that some of the new wound dressings obtained have the potential to significantly reduce (up to 6 logs) both type of bacteria. Further investigation is needed to evaluate the dressing`s potential against bacterial biofilm.

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