International Conference

Processes in Isotopes and Molecules

15th International Conference

PROCESSES IN ISOTOPES AND MOLECULES

Cluj-Napoca, 2025

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Welcome at PIM 2025

It is a pleasure for the National Institute for Research and Development of Isotopic and Molecular Technologies to host the 15th 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 2025 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

From Lab to Field: Advancements in water contaminant detection using portable sensors

S Andreescu

Department of Chemistry and Biochemistry, Clarkson University, Potsdam, NY 13699-5810

E-mail: eandrees@clarkson.edu

Abstract. The presence of contaminants such as pharmaceuticals, personal care products, endocrine disrupting compounds and per/poly-fluorinated substances (PFAS) presents significant challenges to water sources, the environment and human health. PFAS, in particular, are used in commercial products and applications including polymers, fire-retarding foams, cookware and food packaging. Their widespread use poses significant risks due to their high stability, toxicity and tendency to bioaccumulate. This presentation will describe recent work in the development of sensors and analytical technologies for detecting water contaminants, including metal ions, endocrine-disrupting chemicals and the broad spectrum of PFAS, highlighting novel detection mechanisms, analytical performance and potential for low-cost field deployment solutions. The portability of these methods provide opportunities for greater spatial and temporal resolution, enabling more comprehensive characterization and screening of environmental samples. Finally, the presentation will discuss potential applications and critically assess future needs and opportunities for commercialization and translation of these technologies into the practice.

Plenary Pl-2

Metal organic frameworks for critical metal separation

S M Chavan

Department of Chemistry, Bioscience and Environmental Engineering, University of Stavanger, Norway

E-mail: sachin.m.chavan@uis.no

Abstract. Metal-Organic Frameworks (MOFs) have emerged as a highly promising material for various applications. MOF's potential in critical metal separation is a topic of significant interest. Critical metals such as Cobalt, Lithium, Rare earth elements and Platinum group elements play a pivotal role in strategic technologies such as energy, e-mobility, digitalisation and aerospace etc. Due to supply constrained and environmental challenges, ensuring a secure and sustainable supply of critical metals is top priority. Extensive research is carried out to develop efficient technology for extracting critical metals from both the primary and secondary resources. Given the tunability of MOFs with desired functionality, they can serve as an exceptional adsorbent for the separation and purification of metals. MOFsorbMET project aimed at validating the MOFs for critical metal separation and addressing the benefits and limitations. This presentation will discuss our findings from the MOFsorbMET project, highlighting the performance, opportunities and limitations of MOFs particularly for Nickel, Cobalt, Silver and Lithium adsorption separation.

Plenary Pl-3

Computational approaches to study DNA spatial organization in healthy and pathogenic genomes

A M Chiariello

Dipartimento di Fisica, Università degli Studi di Napoli Federico II, and INFN Napoli, Complesso Universitario di Monte Sant'Angelo, 80126 Naples, Italy

E-mail: andreamaria.chiariello@na.infn.it

Abstract. Within the cell nucleus of eukaryotic organisms, chromosomes are organized in a complex, non-random three-dimensional (3D) spatial structure, which is intimately linked to vital functional purposes. Indeed, genome organization regulates the transcriptional activity of genes, as a correct folding allows an efficient communication between genes and their distal regulator elements while, if altered, can cause severe diseases. In this talk I will discuss how theories from Physics, combined with Molecular Dynamics simulation and Machine Learning based inference, represent a powerful tool to quantitatively investigate the complexity of 3D organization of real genomes, as highlighted by recent microscopy and biochemical experiments. Furthermore, I will show that simple physical processes, widely studied in Statistical Mechanics, such as phase-separation of molecular aggregates and coil-globule polymer transitions, allow us to make sense of recent experimental observations including the tissue-specific DNA structure, the structural variability of chromatin at the single cell level and the formation of novel, regulatory-linked architectural conformations. Importantly, polymer models can be used to study the impact of disease-linked genetic mutations or the effect of viral infection such as SARS-CoV-2, opening the way to new potential supporting tools for medical research.

Plenary Pl-4

The major challenge of authenticating the origin of honey: portable spectroscopy for the development of a traceability system

A Mara[1], R Chignola[2], M Migliorini[2] and M Ciulu[2]
[1] Department of Chemical, Physical, Mathematical and Natural Sciences, University of Sassari, Via Vienna 2, 07100 Sassari, Italy
[2] Department of Biotechnology, University of Verona, Strada le Grazie 15, 37134 Verona, Italy

E-mail: marco.ciulu@univr.it

Abstract. The honey sector is one of the most affected by food fraud. These include not only the illicit practice of adding syrups of various kinds but also the falsification of botanical and/or geographical origin. Although some studies show that some fractions of the minority composition of honey can be studied in order to geo-reference samples, the high cost of the techniques used and the long analysis times make the techniques considered so far, although highly performing, unsuitable for the analysis of the large number of samples on the market. For this reason, it is necessary to develop fast, accurate and implementable on-site screening strategies for rapid verification of declared origin. In the present study, which originated as a collaborative activity of WG1 of Cost Action CA22105, it will be described how from a sampling of about 1,000 samples from various geographic areas and of different varieties, it was possible by means of a portable FT-NIR device to lay the foundations for a traceability model of honeys belonging to the European market. The critical aspects of large-scale classification of honeys belonging to a multitude of different areas in comparison with that of honeys belonging to delimited territories will be discussed along with the key role of machine-learning for a positive outcome.

Plenary Pl-5

When Nano Meets Need: Advanced materials for tackling today's water treatment challenges

N Dulova

Tallinn University of Technology, Department of Materials and Environmental Technology, Ehitajate tee 5, 19086 Tallinn, Estonia

E-mail: niina.dulova@taltech.ee

Abstract. The growing global demand for clean water, along with increasing pollution from industrial, agricultural, and municipal sources, emphasizes the urgent need for advanced water treatment solutions. Traditional treatment technologies often fall short in removing contaminants such as persistent organic pollutants, heavy metals, and emerging contaminants. Recent developments in functional nanomaterials including metal-organic frameworks, covalent organic frameworks, carbon-based nanostructures, metal and metal oxide nanoparticles, and tailored nanocomposites, have demonstrated superior performance in adsorption, (photo)catalytic oxidation, membrane filtration, and water disinfection applications. The nanostructured materials offer high surface area, enhanced reactivity, and tunable surface functionalities, significantly improving contaminant removal efficiency. Furthermore, hybrid materials that combine the properties of different components can further enhance treatment performance by enabling target-specific adsorption, improved separation, and material reusability. The application of these advanced materials provides innovative and effective solutions to complex water purification challenges. Continued research and development in this field are essential to address issues such as long-term material stability and environmental safety, and to enhance the sustainability and scalability of these technologies for global use in clean water production.

Plenary Pl-6

Electrospun Nanofiber Coatings: Enhancing corrosion resistance and enabling advanced biosensing

M Florescu[1] and M David[2]

[1] Faculty of Medicine, Transilvania University of Brasov, Brasov, Romania

[2] Faculty of Chemistry, University of Bucharest, București, Romania

E-mail: florescum@unitbv.ro

Abstract. Electrospinning has emerged as a versatile and cost-effective technique for fabricating nanofiber-based coatings with tailored physicochemical properties. This presentation explores the dual functionality of electrospun nanofiber coatings in two critical applications: increasing corrosion resistance and biosensing. By incorporating functional polymers and nanoparticles into the electrospinning process, it is possible to produce highly uniform, porous, and adhesive coatings that act as effective barriers against corrosive agents. The resulting nanostructured layers not only improve the mechanical durability and chemical stability of metallic surfaces but also provide a tunable platform, enabling the integration of biorecognition elements and facilitating the development of sensitive and selective biosensors. The integration of protective and sensing capabilities within electrospun nanofiber coatings offers a promising strategy for multifunctional surface engineering.

Plenary Pl-7

The journey of underground argon: A global infrastructure for dark matter research with the DS-20k experiment

F Gabriele on behalf of DarkSide Collaboration

Istituto Nazionale di Fisica Nucleare, Sezione di Cagliari, Dipartimento di Fisica Complesso Universitario di Monserrato S.P. per Sestu – Km 0,700 09042 – Monserrato (Cagliari), Italy

E-mail: federico.gabriele@lngs.infn.it

Abstract. The DarkSide-20k experiment, designed to detect Dark Matter using a dual-phase liquid argon time projection chamber (LAr TPC), requires a source of ultra-pure, low-radioactivity argon. To meet this need, an integrated infrastructure has been developed for the production and validation of Underground Argon (UAr), involving three key projects: Urania, Aria, and DArT. Urania, located in the United States, is responsible for extracting UAr from deep underground wells and performing an initial chemical purification. The gas is then liquefied for transport to Italy, where Aria—a 350-meter cryogenic distillation column being installed at the Carbosulcis minesite—carries out further purification from chemical contaminants. While its primary purpose is to purify UAr for DarkSide, Aria is also designed for isotopic separation, with broader potential applications in fields such as medicine and nuclear technologies. The final step involves DarT, an argon-filled detector currently operating at the Laboratorio Subterráneo de Canfranc (LSC) in Spain, which validates the UAr by characterizing its radiopurity and performance in detector-like conditions. This vertically integrated production chain is a crucial element for the success of the DarkSide-20k program and represents a significant technological effort with implications for both fundamental research and future commercial and industrial developments.

Plenary Pl-8

Targeted nanostructures for fighting diseases: Strategies against cancer, bacterial infections or ALS

S Gómez-Ruiz

COMET-NANO Group, Departamento de Biología y Geología, Física y Química Inorgánica, E.S.C.E.T., Universidad Rey Juan Carlos, Calle Tulipán s/n, E-28933 Móstoles, Madrid, Spain

Instituto de Investigación de Tecnologías para la Sostenibilidad, Universidad Rey Juan Carlos, Calle Tulipán s/n, 28933 Móstoles, Madrid, Spain

E-mail: santiago.gomez@urjc.es

Abstract. The development of targeted nanostructures has become a powerful strategy to address the challenges associated with the complexity and specificity of modern biomedical therapies. In this talk, the most recent advances from the COMET-NANO group at Rey Juan Carlos University (Spain) will be presented, focusing on the design and functionalization of nanomaterials with therapeutic applications. Specifically, we will discuss the use of porous silica-based and graphene-derived nanostructures functionalized with therapeutic metal complexes or bioactive organic molecules, in combination with targeting ligands such as folic acid, transferrin, triphenylphosphonium salts, or even leptin. These systems are engineered to enhance cellular uptake, target selectivity, imaging capabilities, and therapeutic performance in pathological environments. Their application in three major biomedical challenges, cancer, bacterial infections, and neurodegenerative diseases such as amyotrophic lateral sclerosis (ALS), will be explored. The presentation will cover from the rational design of these multifunctional platforms and their mechanisms of therapeutic action to the final discussion on current challenges and future directions for their potential preclinical advances and their perspectives for clinical translation.

Plenary Pl-9

Advanced laser technologies as tools for spectroscopy

M Guina

Optoelectronics Research Centre, Tampere University, Korkeakoulunkatu 3, 33720 Tampere, Finland

Vexlum Ltd, Kauhakorvenkatu 53B, 33720 Tampere, Finland

E-mail: mircea.guina@tuni.fi

Abstract. The rapid progress of quantum technologies and precision spectroscopy is driving demand for advanced laser sources with unprecedented levels of stability, spectral purity, tailored wavelength coverage, compactness, and user versatility meeting stringent requirements. In general, innovations in semiconductor laser technology are enabling emerging applications that exploit the fundamental interactions of atoms, ions, and molecules, thereby shaping the future landscape of quantum technology applications and spectroscopy.

First, we discuss recent developments of commercial vertical-external-cavity surface-emitting lasers (VECSELs), providing watt-level output power, narrow linewidths, and broad wavelength tunability across the visible and near-infrared range. Then, we focus on recent efforts on developing photonic integration platforms that have enabled on-chip single-frequency lasers with sub-MHz linewidths, which are instrumental for portable spectroscopic systems. Beyond coherent laser sources, progress in superluminescent diodes (SLDs) is pushing the performance envelope of broadband, spatially coherent light emitters. To this end, we review recent demonstrations of SLDs operating beyond 2 µm, which open new possibilities for absorption spectroscopy of molecular species in the mid-infrared “molecular fingerprint” region. Such devices combine the advantages of compactness, robustness, and high brightness, bridging a gap between traditional laser diodes and thermal emitters.

Plenary Pl-10

From ^{13}Clues to ^{18}Origin, ^{2}History and ^{15}N-Profiling — Tracing food authenticity with isotope fingerprints

R E Ionete, O R Botoran, A M Simionescu, and D Costinel

National Research and Development Institute for Cryogenic and Isotopic Technologies-ICSI Rm. Valcea, 4th Uzinei Street, 240050 Rm. Valcea, Romania

E-mail: roxana.ionete@icsi.ro

Abstract. Amid ongoing concerns regarding food fraud and origin misrepresentation, stable isotope ratio analysis has become a reference method in food forensics. This work presents a multi-isotopic approach to food traceability, building on ICSI's experience in the authentication of honey, wine, vinegar, fruit juices, jams, and extending it to tomato-based products—a category increasingly vulnerable to adulteration. The methodology combines several light stable isotopes: $\delta^{13}C$ (botanical origin, sugar addition), $\delta^{15}N$ (agricultural practices, organic vs. conventional inputs), and $\delta^{18}O/\delta^{2}H$ (geographic origin, water source). Special focus is placed on D/H ratio measurements via SNIF-NMR, highly effective in detecting unauthorized water addition or sugar adulteration in fruit juices, wine, and honey. A validation study on tomato juice, paste, and ketchup, using both authentic and commercial samples, confirmed the thermal stability of $\delta^{13}C$ and $\delta^{15}N$, while D/H and $\delta^{13}C$ variations in sugars and ethanol reflected formulation differences. Isotopic signatures of $\delta^{2}H$ and $\delta^{18}O$ helped identify exogenous water addition and discriminate production origins. The study supports the application of multi-isotope profiling for both raw and processed food authentication, while also highlighting the need for regional isotopic databases and isoscapes. Integration into digital traceability and certification systems is discussed as a pathway toward improved food integrity.

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Plenary Pl-11

Transitioning to urban climate neutrality and climate positive cities with the synergy of solar energy technologies and nature-based solutions

D Karamanis, N Skandalos, T Dimitriou

Renewable Energy Sources & Cool Urban Environment, University of Patras, 30100, Agrinio, Greece

E-mail: dkaraman@upatras.gr

Abstract. To facilitate urban transformation and transition away from fossil fuels, climate responsive urban strategies should be urgently applied on a global scale. The accurate knowledge of the effectiveness of sustainable and resilient urban solutions is needed while a convergence solutions framework of implementation should be introduced and optimized across the cities diverse climate conditions. In this work, a novel framework of urban transformation is proposed based on four pillars: green inclusive (reduce), inspirational & recreational (avoid), decisional (replace) and sufficiency, sharing and caring (transition). The synergistic effects of solar energy technologies and greenery are revealed in a customized approach of these solutions implementation through the investigation of energy balance and CO2 emissions for a typical Mediterranean city with poor air quality during winter. As positive climate urban transformation is complex and difficult, an emphasis on the integration of economic and technological dimensions with social inclusion is imperative.

Plenary Pl-12

Perspectives on the use of the pressure-retarded osmosis process for efficient energy storage and power generation

P Łapka, F Dietrich, J Wachnicki and Ł Cieślikiewicz

Warsaw University of Technology, Faculty of Power and Aeronautical Engineering, Institute of Heat Engineering, 21/25 Nowowiejska Str., 00-665 Warsaw, Poland

E-mail: piotr.lapka@pw.edu.pl

Abstract. Pressure-retarded osmosis (PRO) is a membrane-based process that can be used to generate power from the salinity difference between two solutions. The PRO process is typically considered to be implemented using sodium chloride (NaCl) solutions and natural saltwater, since it was originally designed for open system configurations with naturally occurring saltwater sources. However, open configurations using naturally available NaCl solutions do not offer sufficient power density to make the technology economically viable. Therefore, alternative ways of implementing the PRO process for power generation are being investigated. These include using a closed system configuration, various organic and inorganic salt solutions, high-concentration solutions, and an elevated process temperature. This work explores implementing a closed-loop PRO process concept for power generation and thermal energy storage using heat from low-grade waste or renewable sources. Furthermore, it considers the use of alternative synthetic salt solutions with concentrations close to their solubility limits and elevated solution temperatures. To conduct the investigations, a fully automated in-house PRO test bench and an advanced process model were developed. The results of the initial tests and simulations are presented alongside a discussion of the prospects for the PRO process.

Plenary Pl-13

Probing the folding pathway of BS3 β-Lactamase with high structural and temporal resolution

R Malempré[1], J Vandenameele[1], C Montagner[1], C Redfield[2], C Damblon[3], G Mazzuchelli[3], S Brier[4] and A Matagne[1]

[1]Laboratory of Enzymology and Protein Folding, Centre for Protein Engineering, InBioS Research Unit, University of Liège, Liège, Belgium

[2]Department of Biochemistry, University of Oxford, South Parks Road, Oxford, OX1 3QU, United Kingdom

[3]Départment of Chemistry, MolSys Research Unit, University of Liège, Belgium

[4]Biological NMR and HDX-MS Technological Platform, CNRS UMR3528, Université Paris Cité, Institut Pasteur, Paris, 75015, France

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

Abstract. Class A β-lactamases, with their complex architecture and significant size (*ca.* 29 kDa), provide an excellent model for studying key features of protein folding. These enzymes exhibit two particularly interesting structural aspects: the formation of a β-domain with strands contributed by different polypeptide chains and the unique packing of a large Ω-loop on the protein surface. While protein folding studies have traditionally focused on smaller, single-domain proteins with simple folding kinetics, β-lactamases have enabled the exploration of folding intermediates and distinct pathways in larger systems. Using *Bacillus licheniformis* BS3 β-lactamase as a model, we have elucidated the folding process by combining quenched-flow hydrogen/deuterium exchange pulse-labelling with high-resolution techniques such as 2D-NMR and proteolytic fragmentation mass spectrometry. These approaches have tracked the formation and stabilization of secondary structure elements over time and identified folding intermediates. BS3 β-lactamase has proven particularly suitable for such studies due to its high solubility, stability, ease of purification, measurable biological activity, and well-characterized 3D structure at 1.7 Å resolution. The availability of its assigned ^{1}H-^{15}N HSQC NMR spectrum has further facilitated detailed kinetic and structural investigations, offering new insights into protein folding pathways and intermediate states.

Plenary Pl-14

Carboxylate platform for waste valorisation

P Oleskowicz-Popiel

Water Supply and Bioeconomy Division, Faculty of Environmental Engineering and Energy, Poznan University of Technology, Berdychowo 4, 60-965 Poznan

E-mail: piotr.oleskowicz-popiel@put.poznan.pl

Abstract. Human activity is the major driver of climate change which has impact on food production, migration patterns, public health, economic and political stability. At the same time modern societies are losing great amount of carbon in form of organic waste, wastewater and CO_2 which all could be recovered and returned back to the society while preventing or minimizing the use of fossil resources. The future of the current petroleum and chemical industry is in bio-based alternatives. For the bioeconomy to be efficient and cost effective at a large scale, new biotechnologies must be developed and open (mixed) culture fermentation is one of them. Carboxylate platform presents a promising solution for converting wide range of organic waste and wastewater into platform chemicals. Those chemicals can be then upgraded to a variety of commodity products.

Plenary Pl-15

Intrinsic photoanode band engineering for enhanced solar water splitting efficiency in Ti-doped hematite nanorods

D Stănescu[1], Y J. Dappe[1], D Ihiawakrim[2], O Ersen[1], and Ş Stănescu[3]
[1]SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay 91191 Gif-sur-Yvette Cedex, France
[2]IPCMS, CNRS UMR 7504, 23 rue du Loess, BP43, 67034 Strasbourg, France
[3]Synchrotron SOLEIL, L'Orme des Merisiers, 91190 Saint-Aubin, France

E-mail: dana.stanescu@cea.fr

Abstract. Hydrogen production by splitting water molecules into H_2 and O_2 using sunlight is a very attractive idea because it allows storing solar energy in the H_2 molecules using a clean method. First demonstration of water splitting was reported 50 years ago using TiO_2 as photoanode. Since then, plethora of studies were reported, owing to materials scientists' infinite imagination, addressing different classes of photosensitive materials including semiconducting oxides, III-V semiconductors, MOF (metal-organic framework) architectures, ferroelectric materials, etc. Band engineering is additionally often employed targeting each time the same single aim: enhance the efficiency of the photoelectrochemical process, increasing thus H_2 production efficiency. I present a simple band engineering approach applied to one of the most Earth abundant materials, the hematite, using Ti doping and tuning annealing conditions: temperature and gas atmosphere. We found strongly enhanced photocurrent, mediated by surface states, as evidenced by electrochemical impedance spectroscopy. The nanoscale origin of the increased photoelectrochemical activity was addressed using combined XPEEM, STXM, X-rays spectro-ptychography and STEM. Shadow XPEEM alone can be used to discriminate surface and bulk contributions of the chemistry and chemical coordination. STXM complement successfully these results evidencing formation of Ti-rich clusters in the Ti-doped hematite nanostructures annealed in O_2-free atmosphere. Spectro-ptychography allows to better identify and isolate both spatially and chemically Ti-rich clusters. X-ray spectromicroscopies altogether were confronted with STEM measurements and DFT calculations.

Plenary Pl-16

States of the art analytical methods for the structural characterization of natural mixtures

A Tintaru

Aix-Marseille University, CNRS, Centre Interdisciplinaire de Nanoscience de Marseille – UMR7325, 13009 Marseille, France

E-mail: aura.tintaru@univ-amu.fr

Abstract. For several years now, essential oils (EOs) have been attracting growing interest from the public, who invest lavishly in skincare products with exceptional properties. Obtained from aromatic, perfumed and medicinal plants, these complex mixtures made up of dozens of molecules offer a wide range of applications in cosmetics, food processing, aromatherapy, perfumery, medicine, etc. To explore at maximum their beneficial properties, we need to know their chemical, physico-chemical and biological characteristics, and identify the hazards associated with the production, marketing and use of these high added-value products. It has become essential to have a reliable and rigorous analytical sequence capable of gathering the new demands of consumers in terms of quality and safety.

Therefore, for reliable characterization of natural mixtures, each of the constituent products must be described in terms of its concentration, structure and, where appropriate, stereochemistry. Hence, the most challenging issue remains isomers identification and characterization. To do this, combined analytical strategies are used to provide the most detailed possible composition of each studied sample. Today, in addition to the analytical methods traditionally used (GC-MS, LC-MS, SPE, NMR), more modern techniques are being used (ESI-MS, tandem mass spectrometry, ion mobility coupled with mass spectrometry).

In this context, through some practical examples this presentation will illustrate alternative approaches, based on the combination of NMR, ion mobility-mass spectrometry (IM-MS) and quantum chemistry (QM), for the direct isomers' differentiation in crude essential oils and other kind of isomer mixtures.

Keynote K-1

Ultrasensitive photothermal characterization of thermoplasmonics nanoparticles for efficient cancer phototherapy

H Cabrera[1], A Alsadig[2], X Peng[2], L R Loureiro[2], A Feldmann[2], R Hübner[3], M Kubeil[1], M Bachmann[1], L Baraban[1]
[1]The Abdus Salam International Centre for Theoretical Physics, Trieste 34151, Italy
[2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiopharmaceutical Cancer Research, 01328 Dresden, Germany
[3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zenztrum Dresden-Rossendorf e. V., 01328 Dresden, Germany

E-mail: hcabrera@ictp.it

Abstract. In this work, we developed thermoplasmonic nanoconjugates consisting of 20 nm spherical gold nanoparticles (AuNPs) or gold nanostars (AuNSs) as nanocarriers, and (ii) surface-passivated antibody-based fibroblast activation protein (FAP)-targeting modules, used in adaptive chimeric antigen receptor T-cells immunotherapy. The nanoconjugates demonstrated excellent stability and specific binding to FAP-expressing fibrosarcoma HT1080 genetically modified to express human FAP, as confirmed by fluorescence activated cell sorting, immunofluorescence, and surface plasmon resonance scattering imaging. Moreover, the nanocarriers showed significant photothermal conversion after visible and near-infrared irradiation. Quantitative thermal lens spectroscopy demonstrated the superior photothermal capability of AuNSs, achieving up to 1.5-fold greater thermal enhancement than AuNPs under identical conditions. This synergistic approach, combining targeted immunotherapy with the thermoplasmonic nanocarriers, not only streamlines nanoparticle delivery, increasing photothermal yield and therapeutic efficacy but also offers a comprehensive and potent strategy for cancer treatment with the potential for superior outcomes across multiple modalities.

Keynote K-2

Bioinspired nanopore sensors using antibody mimetic technologies

L Movileanu[1,2]
[1]Departments of Physics, Biology, and Chemical and Biomedical Engineering, Syracuse University, Syracuse, New York 13244, USA
[2]BioInspired Institute, Syracuse University, Syracuse, New York 13244, USA

E-mail: lmovilea@syr.edu

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. We address 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. 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. The reporting signal unambiguously distinguishes protein recognition events at single-molecule precision without requiring complex analysis algorithms.

SECTION T1

Stable Isotopes and Emerging Approaches

Oral T1-1

Compound specific isotope analysis of chlordecone during its Fenton advanced oxidation in H_2O_2/Mn_2O_3 system

S-L Badea[1], M-N Verziu[2], P Höhener[3]

[1] Research Center for Studies of Food Quality and Agricultural Products, University of Agronomic Sciences and Veterinary Medicine of Bucharest, 59 Marasti Blvd., 011464, Bucharest

[2] Department of Bioresources and Polymer Science, Advanced Polymer Materials Group, Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica Bucharest, 1-7 Gh Polizu Street, Bucharest, Romania

[3] Aix-Marseille University, Environmental Chemistry Laboratory (LCE), UMR 7376, 3 place Victor Hugo - Case 29, 13331 Marseille, France

E-mail: silviu.badea@qlab.usamv.ro

Abstract. In this study, we investigated the Fenton oxidation of chlordecone in the H_2O_2/Mn_2O_3 system. The advanced oxidation experiments were performed in 500 mL Schott-Duran bottles by adding different amounts of α-Mn_2O_3 nanoparticles (0, 5, 10, 20, 50 and 100 mg) as catalyst. Chlordecone was added from a stock solution in acetone to aqueous solutions of 200 mL at pH 6. The oxidation reaction was performed for 6 hours in an incubator at 30 ℃ and 125 rpm. The aliquots of chlordecone were extracted with 1 mL dichloromethane that contained hexabromobenzene (HBB) as internal standard and analyzed by GC-MS. The results of our study indicate that the maximum removal yield of 61 % for chlordecone was obtained in the bottle with 20 mg α-Mn_2O_3, where the concentration of chlordecone decreased. This decrease in concentration was accompanied by a slight isotope fraction of chlordecone, as its carbon isotope signature changed from -23.7 ± 0.3 ‰ to -23.0 ‰. Overall, our study demonstrated the potential of Fenton reaction with new catalysts in degradation of chlordecone, while the kinetics of the degradation reaction is yet to be optimized.

Oral T1-2

Spectroscopic approaches for analyzing Spirulina dietary supplements

M David, A R Hategan and D A Magdas

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

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

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

Abstract. Spirulina is a dried mass of cyanobacteria consumed by humans and valued for its high protein content, micronutrients, and bioactive compounds. It is found on the market in various formulations, including powders, tablets, capsules, or in functional foods. Despite its growing popularity, there is a lack of standardized regulations and quality control practices that lead to high variability of the Spirulina available on the market. The present study proposes a new methodology for analyzing the composition of Spirulina dietary supplements by using vibrational spectroscopy as a rapid, non-destructive tool. In this regard, infrared, Raman spectroscopy and surface enhancement Raman spectroscopy (SERS) were employed to identify the most suitable approaches for observing the vibrational fingerprint of the essential chemical compounds present in Spirulina samples, including proteins, pigments, carbohydrates, amino acids, minerals, and vitamins. Supervised statistical methods, namely partial least squares discriminant analysis (PLS-DA) were employed in order to process the data and identify relevant compositional markers. The findings support the use of vibrational spectroscopy as a promising, fast, easy-to-use screening method for Spirulina quality control, improving product transparency, regulatory oversight, and consumer safety.

Oral T1-3

Enhancing wine recognition through the fusion of ^{1}H-NMR and Raman spectral data

A R Hategan[1,2], M David[1,2], A Pirnau[1], B Cozar[1], and D A Magdas[1,2]

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

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

E-mail: ariana.hategan@itim-cj.ro

Abstract. Wine represents a product of significant economic and cultural value, yet it remains one of the most frequently counterfeited commodities within the agri-food sector. Common forms of fraud include the wrong declarations of the geographical origin, grape variety, or vintage. While established techniques such as stable isotope ratio analysis have proven valuable for wine traceability, there has been a growing interest in the application of faster and non-destructive analytical methods such as ^{1}H-NMR and Raman spectroscopies for constructing effective wine recognition models.

This study evaluates the potential given by the association of ^{1}H-NMR and Raman spectroscopic data to enhance the performance of wine differentiation models concerning grape variety, production region, and vintage. Given the challenges posed by the high dimensionality of fused spectral data, particular emphasis was given to developing an optimized preprocessing strategy. This involved the identification of the most relevant spectral features from each input data type and for each classification, followed by their concatenation through a mid-level data fusion approach. The constructed models demonstrated outstanding performance, achieving perfect recognition in cross-validation and 100% accuracy in testing for cultivar classification. These findings underscore the benefit of spectroscopic data fusion in improving classification reliability, particularly for cultivar discrimination, where traditional methods like isotope analysis are less efficient.

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Oral T1-4

Investigating the biotransformation of TNT by three different bacterial Species using Compound-Specific Isotope Analysis (CSIA)

S Gupta, Z Ronen and H Siebner

Zuckerberg Institute for Water Research, Jacob Blaustein Institutes for Desert Research, Ben Gurion University of the Negev, Israel

E-mail: zeevrone@bgu.ac.il

Abstract. The compound 2,4,6-trinitrotoluene (TNT) is a widely used explosive that causes significant soil and water contamination. While the transformation pathways of TNT have been well characterized under laboratory conditions, their behavior and environmental impact in the field remain difficult to predict. Isotopic tools offer a promising approach to elucidate these pathways and assess their role in environmental degradation. Although extensive research has focused on the abiotic degradation of nitroaromatic compounds (NACs), data on the isotopic signatures associated with biotic transformations—particularly of TNT—remain limited. In this study, we investigated the carbon and nitrogen isotope fractionation patterns linked to the aerobic biotransformation of TNT by several bacterial strains under varying nutritional conditions. Our analysis integrates isotopic data, metabolite profiles, and genomic information related to potential catalytic enzymes. The identified transformation pathways include (1) reduction of nitro groups, (2) nucleophilic attack followed by reduction of the aromatic ring, and (3) oxidation of the methyl group. The bacterial strains exhibited distinct preferences and efficiencies for each pathway depending on the environmental conditions. These differences enabled us to quantitatively characterize the carbon and nitrogen isotope fractionation associated with each specific transformation route of TNT.

Poster T1-1

Operating a modular random packing testing plant for ^{18}O isotope separation via H_2O vacuum distillation

S Bugeac, C Fort, S Radu, R Puscas and Z Szucs

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

E-mail: stefan.bugeac@itim-cj.ro

Abstract. The newly ^{18}O isotope modular separation plant, designed for versatile testing, has successfully undergone commissioning and setup. It allows for experimentation with various types of random packing, differing in shape and material. A comprehensive monitoring and control system was developed, enabling the column to be operated remotely with any number of modules; each module approximately 1 meter high and equipped with temperature and pressure sensors, water inlet and outlet valves, and a sample port. At the bottom, water evaporation is precisely regulated, while a condenser at the top recirculates water for a complete cycle. With this modular testing plant, the separation performance of different random packings has been effectively evaluated.

Poster T1-2

Advanced profiling of pesticide residues in commercially available potato tubers by GC-FID

F D Covaciu, V Floare-Avram, I Feher and Cs Molnár

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

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

Abstract. This study investigates the detection, identification, and quantification of pesticide residues in 50 potato tuber samples sourced from Romania (household and commercial), Greece, Egypt, France, Hungary, and Poland, available on the Romanian market. Employing a rigorously validated Gas Chromatography with Flame Ionization Detection (GC-FID) method, coupled with the optimized QuEChERS extraction technique, the analysis achieved high sensitivity and precision in detecting multiple pesticide residues simultaneously. Of the 50 samples analyzed, 31 (>60%) contained detectable pesticide residues, with 17 out of 29 targeted pesticides identified. Predominant residues included *beta*-BHC, and heptachlor epoxide, with the exhibiting concentrations up to 41.61 µg/kg in Romanian market samples, exceeding the Maximum Residues Limits (MRLs) of 10 µg/kg. Other notable pesticides detected included chloroneb, *trans*-chlordane, and DCPA methyl ester, reflecting both current and historical pesticide use. The results underscore the persistence of organochlorine compounds in the environment and highlight the robustness of GC-FID as a reliable analytical tool for monitoring pesticide residues.

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Poster T1-3

Aries River: insights from isotopic fingerprints of water and sediments

G Cristea, R Puscas and C Voica

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

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

Abstract. River sediments play a crucial role in shaping aquatic ecosystems, transporting nutrients, contaminants, and trace elements from terrestrial to marine environments. Understanding their composition and origin is essential for assessing environmental quality, erosion processes, and geochemical cycling. Isotopic and elemental analyses have emerged as powerful tools to trace sediment sources, decipher weathering processes, and evaluate anthropogenic impacts. In this context, a preliminary set of 60 water samples were collected over three consecutive months (February-April 2025) and 18 sediment samples along the Aries River, Romania. Regarding water samples, the $\delta^{18}O$ variation range was between -10.5 and -9.3 ‰, while $\delta^{2}H$ values ranged between -69.8 ‰ and -63.3 ‰. Preliminary results obtained from sediments showed a mean value of -28.6 ‰ for the ^{13}C fingerprint of the bulk organic component, while for the inorganic component, the $\delta^{13}C$ and $\delta^{18}O$ signatures range between -7.4 and -1.2 ‰, and from -13.4 to -10.1 ‰, respectively, versus VPDB international standard.

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Poster T1-4

The influence of beverage vessel on migration of potentially toxic elements (PTEs): health risk assessment

A Dehelean[1], G Cristea[1], M Tomoiagă[2], V Mirel[1], S Mirel[3]

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

[2]National College "Emil Racoviță", Cluj-Napoca, Romania

[3] "Iuliu Hațieganu" University of Medicine and Pharmacy, Cluj-Napoca, Romania

E-mail: adriana.dehelean@itim-cj.ro

Abstract. The present study aimed to identify and evaluate the migration of PTEs (Cd, Pb, As, Cu, Ni, Mn, Cr and Al) from diverse FCMs (cups for serving common beverages, having different pH), in real-life scenarios, at different contact times. Then, the study aimed to assess the associated risks, both potentiallly non-carcinogenic and carcinogenic, by consuming some beverages (green tea, green tea with lemon and coffee) served in various types of cups (stainless steel, ceramic, cardboard, and recycled cardboard). After the migration experiment, the beverage samples were collected at different contact times (30 min, 2 hours, and 24 hours), obtaining a total set of 36 samples. The pH, temperature and electrical conductivity were measured. The pH effect is much stronger than the temperature; significant migration was identified for Cd, Pb, Cr. Beverages with an acidic pH and active organic compounds (lemon tea, coffee) favour a higher migration of Cd, Cr and Ni in the first hours of contact. None of the samples posed a non-carcinogenic risk. Regarding carcinogenic risk: none of the samples were in the high-risk interval for Pb; for Cr, 66 % of the samples present very low risk, and 38 % low risk, and Cd, As values posse high risk.

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Poster T1-5

Surface river water evaluation based on ICP-MS content and chemometrics

I Feher[1], C Voica[1], G Cristea[1], A Dehelean[1] and O Marincas[2]

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

[2] Environment Health Center, Part of ALS, 58 Busuiocului Street, 400240 Cluj-Napoca, Romania

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

Abstract. The present study aims to evaluate the chemical content of surface water, with a focus on heavy metals, respectively rare earth elements (REEs). The four important rivers in Romania, which were investigated within this study are: Someș, Mureș, Olt and Prut. Water samples were taken from several representative points for each river and analyzed using Inductively Coupled Plasma Mass Spectrometry (ICP-MS). The experimental data were subjected to rigorous statistical analysis, using analysis of variance (ANOVA) and linear discriminant analysis (LDA), to identify significant differences between rivers. The results revealed significant variations in the concentrations of elements, especially in areas influenced by industrial and agricultural activities. The study's conclusions emphasize the need for continuous monitoring and implementation of water quality protection measures, especially in regions with increased anthropogenic pressure.

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Poster T1-6

Isotopic and multielement characterization of bottled mineral waters on the Romanian market

V Mirel[1], R Puscas[1], C Voica[1], G Cristea[1] and S Mirel[2]

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

[2] "Iuliu Hațieganu" University of Medicine and Pharmacy, Cluj-Napoca, Romania

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

Abstract. Bottled waters are widely consumed globally, not only for hydration but also for perceived purity and health benefits. Their isotopic and elemental compositions provide critical insights into their geographical origin, geological sources, and processing history. In this study, a total set of 56 still mineral water samples were collected, corresponding to four batches from the 14 most widely distributed domestic brands of bottled waters on Romanian market. IRMS and ICP-MS were used as analytical techniques. The hydrogen (δ^2H) and oxygen ($\delta^{18}O$) isotope ratios of Romanian bottled water samples ranged from -79.2 ‰ to -70.0 ‰, and between -11.6 ‰ and -10.4 ‰, respectively. The obtained isotopic signatures fall in the normal range for meteoric waters, clustering along the meteoric water line. The range of macro-element concentrations was: Na: 0.905–275.62 mg/L; Mg: 0.109–93.143 mg/L; K: 0.125–27.231 mg/L and Ca: 5.32–128.601 mg/L. According to the EU classification (80/778/EEC and 2003/40/EC), 4 % of the analyzed bottled waters may be classified as "containing sodium" and 77 % were "suitable for low sodium diets." Variability among bottled water brands often mirrors the heterogeneity of natural aquifers and the distinct geological settings from which they are drawn.

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Poster T1-7

Optimizing Separation Efficiency: Hydrophilicity analysis of random packing

S Radu, C Lar, A Balla, C Varodi, S Bugeac, J Z Szücs-Balázs

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

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

Abstract. The evaluation of surface hydrophilicity is essential for various scientific and industrial applications. In this study, the contact angle method was employed to assess hydrophilicity, and a novel measurement device was designed and fabricated to enhance precision. The system integrates a digital microscope coupled with dedicated software, enabling accurate contact angle determination. This innovative approach improves measurement reliability and provides a valuable tool for characterizing surface wettability.

Poster T1-8

Metal-oxide nanocomposite biochar functionalized for grey water decontamination

J Nzeh, D Gidey, R Bernstein, Z Ronen

Zuckerberg Institute for Water Research, The Jacob Blaustein Institutes for Desert Research, Ben Gurion University of the Negev, Beersheba 8499000, Israel

E-mail: zeevrone@bgu.ac.il

Abstract. Greywater is wastewater generated from domestic activities such as bathing, laundry, and dishwashing, excluding toilet waste. Greywater is a potential alternative water source for sustainable irrigation. However, it typically contains micropollutants that can negatively affect plants and soil when used for irrigation. It also contains antibiotic-resistant bacteria (ARB) and resistance genes (ARGs), which are potentially harmful to humans and the environment. This research developed a low-cost metal oxide (MO) nanocomposite biochar (NC-BC) with enhanced adsorption and catalytic properties for removing ARB and ARGs from greywater. The biochar was produced from sewage sludge by pyrolysis and then activated with NaOH to increase its surface area. Bismuth oxide and ferric oxide nanoparticles were incorporated into the biochar using either a one-pot or two-step method. The material was characterized using various techniques, such as BET, SEM, FTIR, XRD, and XPS. Its adsorption and catalytic activity were studied under different wavelengths using methyl blue as a model compound and DNA as a model for ARG using synthetic greywater. The results showed that the incorporation of the nanoparticles into the biochar significantly enhanced its adsorption capacity and introduced photocatalytic activity. This material is currently being investigated for the removal of ARB and ARGs from real greywater.

Poster T1-9

Comparative efficiency analysis of molecular oxygen cryogenic distillation vs. water distillation for oxygen-18 separation

J-Zs Szücs-Balázs[1], A Balla[1], S Bugeac[1], C Lar[1], C Marcu[1], S Radu[1], C Varodi[1], F Gabriele[2]

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

[2] National Institute for Nuclear Physics (INFN), Cagliari Division, 09042 Monserrato (Cagliari), Italy

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

Abstract. The production of oxygen-18 (^{18}O) is crucial for various applications in medicine, environmental science, and industry. This study presents a comparative analysis of two prominent methods for ^{18}O enrichment: cryogenic distillation of molecular oxygen (O_2) and distillation of water (H_2O). We evaluate the efficiency of these methods based on separation factors, energy consumption, and production yields. The comparison focuses on the theoretical foundations and operational parameters of both methods, highlighting key differences in their implementation and performance.

Poster T1-10

Ecological risk assessment of heavy metal pollution along Aries River

C Voica[1], A Dehelean[1], G Gati[2], and O Marincas[2]

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

[2] Environmental Health Center – Part of ALS, 58 Busuiocului, 400240, Cluj-Napoca, Romania

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

Abstract. Water quality and security are critical for achieving the United Nations Sustainable Development Goals (UN, 2020). The Aries River catchment in northeastern Romania is significantly affected by mining-related pollution of historic origin and current activities, including tailing deposits, decantation ponds, most of them decommissioned, and contaminated mine water—sources of heavy metal contamination that persist beyond active mining. This study evaluates surface water quality in the Aries River catchment, focusing on areas influenced by mining, using various heavy metal pollution indices. The mean concentrations of heavy metals (mg/L) were: Fe (1.967), Mn (0.945), Sr (0.207), Ti (0.162), Zn (0.108), Cu (0.047), Ba (0.027), and As (0.016). Ecotoxicological assessment methods were applied to evaluate the ecological risks posed by these contaminants. The findings highlight that both historical and ongoing mining activities have significantly altered the river's water chemistry, posing risks to environmental and human health.

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SECTION T2

Molecules, Biomolecules and Photonics

Oral T2-1

Determination of the Optimal Dose of Superabsorbent Hydrogel to Mitigate Drought Stress in Bean (*Phaseolus vulgaris* L.)

H Y Dasgan [1], A Keskin[1], B Ikiz [1] and M L Soran[2]

[1]Department of Horticulture, Faculty of Agriculture, University of Cukurova, Adana 01330, Türkiye

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

E-mail: dasgan@cu.edu.tr

Abstract. Under abiotic stress conditions, hydrogel polymers with the ability to retain water and nutrients have become a significant focus of research. Similarly, the addition of biochar is also known to support plant growth under such stress conditions. In this study, the effects of superabsorbent hydrogel (SAH) composed of alginate-based hydrogels and biochar derived from plant peels, applied at different doses, on the cultivation of beans (*Phaseolus vulgaris* L.) under drought stress were investigated. Six different treatments were employed: control, drought, drought + 0.5 g SAH, drought + 1.5 g SAH, drought + 2.5 g SAH, and drought + 3.5 g SAH. Drought stress adversely affected the morphological and physiological characteristics of the plants. However, it was determined that SAHs, applied at different doses, mitigated the adverse effects of drought on physiological parameters such as relative leaf water content, stomatal conductance, leaf water potential, and chlorophyll content. Notably, the application of 2.5 g SAH significantly reduced MDA levels. SAHs were found to strengthen the antioxidant defense system in plant tissues under drought stress, thereby reducing oxidative damage. This effect was associated with increases in phenolic and flavonoid components, as well as activities of proline, ascorbate peroxidase (APX), glutathione reductase (GR), and superoxide dismutase (SOD). Furthermore, SAHs alleviated the negative effects of drought on growth parameters, such as plant weight, root length, root weight, and leaf number.

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Oral T2-2

Spectroscopic and electrochemical approach to characterize the interaction between biologically synthesized nanoparticles and PFAS contaminants

M David[1], M Florescu[2] and C Bala[1,3]

[1] Laboratory for Quality Control and Process Monitoring, University of Bucharest, 4-12 Elisabeta Blvd.,030018 Bucharest, Romania

[2] Department of Fundamental, Prophylactic and Clinical Disciplines, Faculty of Medicine, Transilvania University of Brasov, 1 Universitatii Str, 500068 Brasov, Romania

[3] Department of Analytical Chemistry and Physical Chemistry, University of Bucharest, 4-12 Elisabeta Blvd.,030018 Bucharest, Romania

E-mail: melinda.david@s.unibuc.ro

Abstract. Nanotechnology is a key driver of scientific progress, with increasing emphasis on the use of nanomaterials. Recently, the focus has shifted from physical and chemical synthesis methods to biological approaches. Biological synthesis offers distinct advantages, leveraging the functional groups present in plant extracts. Active compounds in these extracts act as reducing and stabilizing agents, enabling the tailored functionality of nanoparticles while reducing energy consumption, minimizing the use of hazardous chemicals, and lowering production costs. Herein, biologically synthesized gold nanoparticles (AuNPs) are employed for the electrochemical detection of per- and polyfluoroalkyl substances (PFAS). PFAS are persistent environmental contaminants commonly found in water supplies and food, often referred to as "forever chemicals" due to their chemical stability and resistance to degradation. The interaction between AuNPs and PFAS was first investigated using UV-Vis spectroscopy, followed by quantitative analysis through AuNP-modified electrochemical sensors. Under laboratory conditions, a limit of detection of 0.64 nM was achieved for perfluorooctane sulfonate (PFOS), demonstrating the potential of this method for sensitive PFAS monitoring.

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Oral T2-3

Study of dopamine photochemistry behaviour

A A Farcas, A Bende and A Farcas

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

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

Abstract. The equilibrium geometries and light absorption characteristics of dopamine (DA) and dopamine-o-quinone (DAQ) adsorbed on graphene surfaces were examined using ground-state and linear-response time-dependent density functional theories. Two types of graphene systems were studied: a rectangular form of the hexagonal lattice with optimized C–C bond lengths, serving as a model for graphene nanoparticles (GrNP), and a similar system with fixed C–C bonds at 1.42 Å, representing a graphene 2D sheet (GrS). Analysis of vertical excitations revealed three main types of electronic transitions: those localized on graphene, those localized on DA or DAQ, and charge transfer (CT) transitions. In the case of the graphene–DA complex, the charge transfer excitations exhibited a molecule-to-surface (MSCT) character, while for the graphene–DAQ complex, the charge transfer was of the reverse type, surface-to-molecule (SMCT). This difference arises from the presence of a low-lying unoccupied orbital (LUMO+1) in DAQ, which facilitates charge transfer from the surface to the molecule.

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Oral T2-4

In vivo and in vitro ^{1}H NMR imaging, relaxometry and spectroscopy at 11.7 T using INSPIRE – Cluj-Napoca infrastructure

R Fechete[1,2], R Crainic[1,2], M R Băcilă[3], A Fărcășanu[1,4], L Chiriac[1,5], D Petrișor[1], B Frențiu[1], S Simon[1]

[1] Babes-Bolyai University, Institute for Interdisciplinary Research in Bio-Nano-Science, Preclinical MRI Centre (INSPIRE platform), Cluj-Napoca, Romania

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

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

[4] Amethyst Radiotherapy Center, Cluj, Romania

[5] Iuliu Hațieganu University of Medicine and Pharmacy, Department 2, Cluj-Napoca, Romania

E-mail: radu.fechete@ubbcluj.ro

Abstract. High field magnetic resonance (MR) imaging, relaxometry and spectroscopy has become an important tool for non-invasive and non-destructive preclinical investigation from living small animals such as mouses, rats or other rodents, for the investigation of various biological materials such as tissues and organs (healthy or with injuries or affected by tumours) or for the characterization of various other types of materials containing hydrogen. At 11.75 T, the magnetic field available at INSPIRE – Cluj-Napoca infrastructure, the MR images present an enhanced resolution and can be used natively or as input for parameter maps such as T_1 or T_2 parametric maps. For that, the acquisition of large series (64 or hundreds) of images with different echo time (TE) or recycle delay (TR – time of repetition) allow, with an appropriate processing procedure, or: i) the acquisition of specific CPMG decays (or saturation recovery build-up) curves which can be analysed using the inverse Laplace inversion to obtain the corresponding spin-spin or spin-lattice relaxation times distributions; or ii) T_1, T_2 and ^{1}H spin density parametric maps. The specific shape of the relaxation curves, observed for the first time using the 11.75 T Bruker BioSpin scanner and ParaVision 360 v.3.5 software allowed us to propose a new kernel in the inverse Laplace inversion which was used to discriminate between the NMR signal originating from water compartments of rat brain located in myeline, intra and inter-cellular. *In vivo* (and *ex vivo*) mouses with back tumour and advanced biomaterials used for the bone regeneration investigated by localized ^{1}H NMR spectroscopy will be discussed.

Oral T2-5

Physical principles of protein phase-separation action on DNA folding associated to pathogenic gene activation

A Fontana and A M Chiariello
Dipartimento di Fisica, Università degli Studi di Napoli *Federico II*, and INFN sezione di Napoli, Complesso Universitario di Monte Sant'Angelo, 80126 Napoli, Italy

E-mail: andrea.fontana@unina.it

Abstract. Phase-separation of proteins resulting from genetic mutations has been shown to trigger aberrant chromatin looping, contributing to disease development, including cancer. However, the physical mechanisms regulating these processes remain unclear. In this study, we employ polymer physics models of chromatin to investigate the relationship between protein self-aggregation and chromatin structure. We show that a simple model, including only protein-protein and protein-chromatin interactions, effectively explains the aberrant looping around certain oncogenes in cells expressing the NUP98-HOXA9 chimeric protein, commonly found in leukemia. Finally, leveraging on our numerical simulations, we compare our findings with experimental data and show that phase-separation properties of chimeric proteins can be harnessed to prevent aberrant gene-regulator contacts.

Oral T2-6

Synthesis and Physicochemical Profiling of Polydopamine- and Cellulose-Modified Hyaluronic Acid Hydrogels for Wound Dressing Applications

I G Grosu[1], I T Varga-Kocsis[1,2], I Kacso[1], A Simion[1], R Gherman[1] and X Filip[1]

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

[2] Facultatea de Biologie și Geologie, Universitatea Babeș-Bolyai, Str. Gheorghe Bilaşcu nr.44, RO-400015, Cluj-Napoca, România

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

Abstract. Millions of skin injuries occur annually due to physical or thermal trauma, and if improperly managed, they may develop into chronic wounds. Hyaluronic acid (HA), plays a central role in all wound healing phases through its involvement in modulating inflammation, promoting cell migration and proliferation, and enhancing angiogenesis. Due to HA's inherent biocompatibility, biodegradability, and hydrophilicity, HA-based hydrogels have emerged as promising wound dressing materials. Hydrogels provide a moist, protective environment while also enabling controlled delivery of therapeutic agents and facilitating tissue regeneration. However, HA-based wound dressings often exhibit inadequate mechanical stability and suboptimal biodegradation profiles, limiting their therapeutic efficacy. This study investigates the enhancement of HA hydrogels through polydopamine (PDA) and cellulose derivatives conjugation, which improves adhesion, biocompatibility, antioxidant properties thereby reinforcing the hydrogel matrix. Different synthetic strategies were explored for the development of hybrid hyaluronic acid-based hydrogels incorporating polydopamine and cellulose derivatives. The resulting hydrogels were comprehensively characterized to assess their structural integrity (solid-state NMR), thermal behaviour (DSC), morphology (electron microscopy), and viscoelastic properties. The hydrogels will further be investigated in terms of biological activity.

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Oral T2-7

Spectroscopic and photophysical Investigation of 1,3-Diphenylisobenzofuran (DPBF): Experimental and theoretical approaches

S Stan[1], J P Prates Ramalho[2,3,4] and V Chis[1,5]

[1] Faculty of Physics, Babeș-Bolyai University, Str. M. Kogălniceanu 1, RO-400084 Cluj-Napoca, Romania

[2] Department of Chemistry, School of Science and Technology, University of Évora, Rua Romão Ramalho 59, 7000-671 Évora, Portugal

[3] LAQV, REQUIMTE, University of Évora, Rua Romão Ramalho 59, 7000-671 Évora, Portugal

[4] Hercules Laboratory, University of Évora, Palácio do Vimioso, Largo Marquês de Marialva 8, 7000-809 Évora, Portugal

[5] Institute for Research, Development and Innovation in Applied Natural Sciences, Babeș-Bolyai University, Str. Fântânele 30, RO-400327 Cluj-Napoca, Romania

E-mail: stefan.stan@ubbcluj.ro

Abstract. 1,3-Diphenylisobenzofuran (DPBF) is a widely used fluorescent probe for singlet oxygen ($^1O_2$) detection in photodynamic applications. In this work, we present an integrated experimental and theoretical analysis to describe its spectroscopic, photophysical and reactive properties in ethanol, DMSO, and DMF. UV-vis and fluorescence measurements across a wide concentration range show well-resolved $S_0 \rightarrow S_1$ electronic transition of π-π* nature with small red shifts in polar aprotic solvents. Fluorescence lifetimes increase slightly with solvent polarity, showing stabilization of the excited state. The 2D PES and Boltzmann populations analysis indicate two co-existing conformers (C_s and C_2), with C_s being slightly more stable at room temperature. TD-DFT calculations were performed using several functionals and the 6-311+G(2d,p) basis set to calculate absorption/emission wavelengths, oscillator strengths, transition dipole moments, and radiative lifetimes. Overall, ωB97XD and cam-B3LYP provided the best agreement with experimental data for the photophysical parameters across all solvents. The photophysical behaviour of DPBF upon interaction with $^1O_2$ can be explained by a small barrier, two-step reaction pathway that goes through a zwitterionic intermediate, resulting in the formation of 2,5-endoperoxide. This work explains the photophysical properties and reactivity of DPBF, therefore providing a solid basis for future studies involving singlet oxygen.

Poster T2-1

In vivo and *ex vivo* effects of rat brain and tumor fixation in formalin evaluated by 11.75 T high field MR imagining, spectroscopy and relaxometry

M R Băcilă[1], A Roman[2], O Bălacescu[2], E Páll[2], M Vasilescu[1], R Fechete[3]

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

[2] Department of Radiology, Prof. Dr. Ion Chiricuta Oncology Institute, 400015 Cluj-Napoca, Romania

[3] Babes-Bolyai University, Institute for Interdisciplinary Research in Bio-Nano-Science, Preclinical MRI Centre (INSPIRE platform), Cluj-Napoca, Romania

E-mail: bacilaroxana15@gmail.com

Abstract. Preclinical magnetic resonance (MR) investigations have become more informative than the simple acquisition of a qualitative MR image. In this sense, *in vivo* and *ex vivo* MR spectroscopy and relaxometry can provide quantitative information about structure and dynamics of biological tissues and organs. In particular, identification and characterization of tumoral tissues is of a great importance. A B16-F10 tumor type was grown near to the backbone of laboratory Mouse, for 7 days and investigated *in vivo*. Then *ex vivo* investigation of organs (tumor, mouse brain and liver) fixed in formalin was performed at regular time intervals up to several months. These assumed T1 and T2 weighted MR imaging, ^{1}H localized NMR spectroscopy (with water saturated protocol) and based relaxometry. For this, a series of 64 images (weighted with the eco time, TE, increased in equal steps) were recorded and analysed. From each voxel, a series of 64 CPMG echo train decay was measured and the corresponding T_2– distribution was obtained by invers Laplace transform. A number of two (*in vivo* tumoral tissue) or three (*in vivo* healthy tissue) resolved peaks have been identified in the T_2– distribution. As, expected, large variation presents the *ex vivo* distribution of transverse relaxation time, T_2. A slight shift towards small T_2– values was observed with the increase of time for formalin fixation. *In vivo* ^{1}H NMR spectra of tumor (and healthy tissue) are reach in information compared to the corresponding spectra recorded for the formalized organs. Additionally, a series of T_2-parametric maps were obtained and used for the characterization of in vivo and ex vivo characterization of Mouse organs (brain and liver) and tissues (with tumor and healthy). Advanced MRI techniques applied in high field (11.75 T), such as imaging, Fourier and Laplace spectroscopy and T_2 parameter maps proved to be important tools for the characterization of tumoral tissues as well as for the evaluation of the effect of formalin fixation.

Poster T2-2

A complementary theoretical study on 6-nitro BIPS spiropyran photo-switching mechanism

Zs Bálint[1,2] and A Bende[1]

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

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

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

Abstract. The photochromic interconversion between spiropyran (SP) and merocyanine (MC) has been investigated by means of Density Functional Theory (DFT) and its linear response time-dependent (LR-TDDFT) version. Molecular configuration of equilibrium and transition geometries in both ground and electronic excited state were obtained considering the ωB97X-D3BJ exchange-correlation (XC) functional together with empirical dispersion correction scheme and using the def2-TZVPP triple-ζ basis set. Conical intersection geometries were located considering the spin-flip TDDFT computation scheme. The most relevant molecular configurations regarding the equilibrium, transition state and conical intersection geometries during the interconversion between SP and MC were mapped and the energetically most favorable relaxation pathways were drawn.

Poster T2-3

Comparative biochemical analysis of protein profile in marketable and non-marketable Romanian potato tubers

P Bulieris[1], A Baciu[2] and A Anghel [3]

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

[2] Potato Research and Development Station, 15 Orban Balazs, 525400, Targu Secuiesc, Romania

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

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

Abstract. Potato tubers that do not meet marketability criteria can account for up to 30% of regular crops and are frequently underutilized, despite their potential as raw materials for functional ingredients. In this study, we analysed ten Romanian potato varieties, including both marketable and non-marketable tubers, to assess their protein profiles. Protein concentration determination and analysis of electrophoretic migration enabled comparative evaluation across all ten varieties. The results indicate that non-marketable tubers exhibit protein levels and migration patterns comparable to those of standard marketable varieties. These findings suggest that non-marketable tubers represent a viable alternative source of high-quality protein, supporting their valorisation within sustainable processing streams and bio-based product development. Moreover, this comparative approach allows for the identification of varieties best suited for such applications.

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Poster T2-4

Blue nanoplastics detection by SERRS: insights from molecules to single-nanoplastic particle detection

I Cârdan[1,2], S C Pînzaru[2], V Zani[3], A M M Gherman[1], R Signorini[3], R Pilot[3], L Barbu-Tudoran[1] and C Farcău[1]

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

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

[3] Department of Chemical Sciences and INSTM Research unit, University of Padova, Padova, Italy

E-mail: ioana.cardan@itim-cj.ro, cosmin.farcau@itim-cj.ro

Abstract. Nanoplastics (NPs) pose an increasing concern due to their widespread environmental presence and potential risks to human health and ecosystems, prompting the development of advanced detection techniques. Among these, surface-enhanced Raman scattering (SERS) spectroscopy is gaining attention for its high sensitivity. While SERS has proven effective for molecular analytes, its application for NPs detection is still being investigated. Moreover, the detection of secondary NPs is particularly challenging due to their diverse sizes, shapes and compositions, as well as the degradation they undergo from prolonged environmental exposure. In this study, we address two key challenges related to the SERS-based detection of secondary NPs. First, we investigated whether SERS substrates optimized for molecular analytes are also effective in detecting individual NPs. Second, we demonstrated the detection of secondary NPs by combining SERS with resonance Raman (RR) spectroscopy. Specifically, we have detected secondary blue NPs by leveraging the RR signal of copper phthalocyanine (CuPc), a pigment commonly used in blue plastics, and by using customized SERS substrates. These findings offer valuable insights into the applicability and limitations of SERS for NPs detection.

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Poster T2-5

Towards chemical accuracy in the excitation energies of O_2 and O_3 molecules

S Stan, C Crăciun, and V Chiş

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

E-mail: vasile.chis@ubbcluj.ro

Abstract. In this work, we employ *ab initio* quantum chemical methods to investigate the vertical excitation energies to the first two singlet excited states of the O_2 and O_3 molecules. For molecular oxygen, calculations are performed at the MRCI+Q level, while for ozone, both STEOM-DLPNO-CCSD and MRCI+Q methods are employed to ensure reliability and consistency. A series of four correlation-consistent basis sets - ano-pVXZ (X = D, T, Q, and 5) is used for each system. Excitation energies to the first two singlet excited states are computed with all basis sets and subsequently extrapolated to the complete basis set (CBS) limit using an exponential scheme. The extrapolated values are then compared with available experimental data. The goal is to assess the performance and convergence behaviour of high-level quantum chemical methods in accurately predicting excitation energies of small yet electronically challenging open-shell and multi-reference systems such as O_2 and O_3.

The results demonstrate that, with proper treatment of dynamic and static correlation effects, chemical accuracy can be attained, providing reliable benchmarks for future theoretical and spectroscopic investigations.

Poster T2-6

Flexible and tunable nanoimprinted gratings covered with metallic thin films for ultrasensitive SERS detection

A Colniță[1], I Brezeștean[1], N E Dina[1], A S Tătar[1], M Suciu[1,2], L Barbu-Tudoran[1,2], V Toma[3] and D Marconi[1]

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

[2] Electron Microscopy Centre, Babeș-Bolyai University, 5-7 Clinicilor St., 400006 Cluj-Napoca, Romania

[3] Faculty of Biology and Geology, Babeș-Bolyai University, 44 Gh Bilaşcu St. 400015 Cluj-Napoca, Romania

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

Abstract. The exploitation of metal-based periodical nanostructures as plasmonic surfaces has led to a new class of surface-enhanced Raman scattering (SERS)-active substrates with high structural homogeneity and signal reproducibility highly sought-after for recent SERS applications. We employed "top-down" and "bottom-up" approaches, such as nanoimprint lithography, magnetron sputtering and pulsed laser deposition to fabricate tunable metallic/ZnO@metallic nanotrenches to detect environmental contaminants (such as crystal violet), toxins and ultimately dopamine (DA), a relevant biomarker of Parkinson's disease (PD). As a preclinically direct application, we investigated spiked, artificial cerebrospinal fluid samples in order to detect low DA concentrations in simulated biological fluids. Furthermore, healthy and PD's induced-mouse striatum and cortical samples were analyzed for ELISA-based estimation of α-synuclein and DA levels, in combination with a SERS/PCA assessment. The developed SERS nanostructured platforms have demonstrated excellent features, such as a limit of detection of 10 pM and analytical enhancement factors up to 10^6.

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Poster T2-7

Comparison of colloidal crystals formed through Stop&Go versus standard convective self-assembly

D Cuibus, C Farcau

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

E-mail: denisa.cuibus@itim-cj.ro, cfarcau@itim-cj.ro

Abstract. Two-dimensional (2D) colloidal crystals offer immense potential for various functional uses, especially in optical devices that capitalize on their distinct morphology and optical properties. Here we investigate the use of Stop&Go convective self-assembly (SG-CSA) variant for achieving high-quality 2D colloidal crystal films. To this aim, the deposition of aqueous suspensions of 600 nm polystyrene spheres on glass substrates is performed using the Stop&Go convective self-assembly method, while also comparing it to the conventional convective self-assembly approach. By analyzing optical images and microscopic transmittance/reflectance spectra, the morphology and optical behaviour of the prepared self-assembled colloidal photonic crystals were characterized.

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Poster T2-8

Effects of hydrogels on beans (*Phaseolus vulgaris* L.) growing under salt stress

H Y Dasgan[1], K Zikaria[1], B Ikiz[1] and M L Soran[2]

[1]Department of Horticulture, Faculty of Agriculture, University of Cukurova, Adana 01330, Türkiye

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

E-mail: dasgan@cu.edu.tr

Abstract. Hydrogel polymers have garnered significant interest for their potential to improve water and nutrient retention under abiotic stress conditions. Similarly, the incorporation of biochar can enhance plant growth and development under such stresses. This study investigated the effects of a superabsorbent hydrogel (SAH), composed of alginate-based hydrogel and biochar derived from fruit peels, on common bean performance under salt stress. The experiment involved six treatments: T1 (control), T2 (salt), T3 (salt + 0.5 g SAH), T4 (salt + 1.5 g SAH), T5 (salt + 2.5 g SAH), and T6 (salt + 3.5 g SAH). Salt stress adversely affected plant morphological traits (e.g., plant height, leaf area, root length), physiological traits (e.g., photosynthesis, stomatal conductance, leaf temperature), nutrient uptake, and water absorption. Additionally, salt stress increased reactive oxygen species (ROS) concentrations, leading to enhanced lipid peroxidation and cellular damage. Treatment T3, which included 0.5 g of SAH, mitigated the effects of salt stress by improving root length, root fresh weight, shoot fresh weight, leaf area, number of leaves, leaf water potential, and stomatal conductance. T3 also enhanced water uptake, reduced membrane damage, and decreased sodium and chloride uptake. This treatment resulted in the lowest lipid peroxidation and the highest proline content, along with increased antioxidant enzymatic activity. Based on these findings, it can be concluded that the application of 0.5 g SAH could improve common bean growth and development under salt stress conditions. Since increasing doses of SAH cause Na accumulation in the root, the salt damage-reducing effect may not have been seen with increasing SAH doses.

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Poster T2-9

Advancing Gene Therapy: An AI-driven computational framework for optimizing polymer-based nanoplatforms in personalized medicine

A A Farcas[1], B Belean[1], L Jánosi[1], L G Parajdi[1,2], I Tóth[1], A Farcas[1]

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

[2] Department of Mathematics, Faculty of Mathematics and Computer Science,"Babes-Bolyai" University, 400084, Cluj-Napoca, Romania

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

Abstract. Recent advancements in gene therapy have marked a transformative milestone in the development of novel therapeutic modalities and have laid the groundwork for next-generation biotechnologies. The efficacy of gene therapy is critically contingent upon the deployment of robust gene delivery systems. Within this context, both natural and synthetic macromolecules serve as fundamental constituents of soft nanotechnology, facilitating the design of delivery vectors with tailored compositions and functionalities. Herein, we introduce a novel computational framework aimed at the optimization of polymer and/or nanocomposite architectures as efficacious constituents for polymer-based nanoplatforms (PBNs). These PBNs are conceptualized as essential scaffolds for transitioning from conventional drug and gene delivery methodologies toward personalized therapeutic strategies. By integratively employing advanced artificial intelligence techniques and modeling approaches, we successfully enhanced the adaptive design process of these polymeric nanoplatforms, leading to synergistic improvements in their performance and applicability.

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Poster T2-10

An exploration of human γD-crystallin affinity for potential aggregation inhibitors

C G Floare, A Pirnau, M Mic and E Matei

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

E-mail: calin.floare @itim-cj.ro, elena.matei@itim-cj.ro

Abstract. Cataract, the leading cause of blindness worldwide, is characterized by the presence of a cloudy area in the eye lens resulting in a loss of transparency. A number of mechanisms contribute to the longevity and transparency of the 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. With advancing age, progressively, or due to some mutations, this fragile equilibrium can be perturbed, causing γ-crystallin insolubilization, misfolding, fragmentation and aggregation.

In this study, we performed a comparative molecular docking analysis of several experimentally investigated molecules of natural origin, that 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. Thirteen phytochemicals were investigated as potential inhibitors of γD-crystallin aggregation, and we compared their binding energies with those of lanosterol, an ingredient present in over-the-counter eye products, to prevent cataracts. We found that the binding energies of lanosterol outcompete those of all the other investigated potential natural inhibitors. We currently started a more precise analysis using molecular dynamics.

Poster T2-11

QuEChERS combined with UHPLC-PDA for quantification of pesticide residues in potatoes

C V Floare-Avram, F D Covaciu, I Feher and Cs Molnár

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

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

Abstract. The aim of our study was to use the Quick Easy Cheap Effective Rugged and Safe (QuEChERS) sample preparation method and ultra-high-performance liquid chromatography coupled to photodiode array detector (UHPLC-PDA) technique for the simultaneous quantification of 14 pesticides from several classes in 50 potato tuber samples sourced from Romania (household and commercial), Greece, Egypt, France, Hungary, and Poland, available on the Romanian market. Of the 14 pesticides analysed using UHPLC-PDA, only six residues: imazalil, fludioxonil, propiconazole, pendimethalin, etoxazole, and clofentezine were detected across the 50 potato samples. The most frequently detected compounds were imazalil, fludioxonil, propiconazole, and pendimethalin, reflecting their common use in potato cultivation and post-harvest treatments. Fludioxonil and pendimethalin were present in all samples, consistently below MRLs, while propiconazole exceeded its MRL (0.01 mg/kg) in 35 samples (70%) with concentrations ranging from moderate to significantly elevated levels. Imazalil appeared in 16 samples (32%), all exceeding the MRL (0.01 mg/kg), with the exhibiting concentrations up to 375.41 µg/kg in Romanian market samples, suggesting possible post-harvest misuse or contamination during storage.

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Poster T2-12

A Neural Network Approach to Surface Enhanced Raman Spectroscopy Substrate Optimization

A M M Gherman[1], M Cristea [2] and C Farcau[1]

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

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

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

Abstract. Surface Enhanced Raman Spectroscopy (SERS) is a highly sensitive and selective detection method that has a vast array of applications in surface and interface chemistry, catalysis, nanotechnology, biology, biomedicine or environmental analysis. Maximizing the SERS signal is of great interest and can generally be done by developing SERS substrates that have a local surface plasmon resonance (LSPR) matching the laser wavelength. In this view, artificial neural networks combined with optimization techniques can be extremely useful tools for providing specific SERS substrate parameters needed for obtaining plasmonic structures with desired plasmon resonances for maximum SERS signal. Thus, in this work we propose optimizing the properties of a periodically structured plasmonic system by employing an artificial neural network that can predict, with high accuracy, the mean electric field at the surface of the nanostructured material which is irradiated with a 785 nm wavelength. The considered periodic structure is silver coated polystyrene nanospheres monolayer, and the parameters that mostly influence the SERS signal, and therefore are optimized, are the polystyrene sphere radius and the thickness of the silver film.

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Poster T2-13

Potential of mean force calculations highlight the energetics behind lignin derivatives' interactions with skin-like membrane

L Janosi[1] and A Farcas[1]

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

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

Abstract. Lignin, a natural and abundant biopolymer, holds significant potential in healthcare and cosmetic products due to its antioxidant, antimicrobial, and anti-inflammatory properties. In this study, we employed free energy calculations on designed small lignin derivatives composed of syringyl and guaiacyl units. Specifically, we used the non-equilibrium so-called FR-method to calculate the potential of mean force along these derivatives insertion into the ceramide bilayer along the normal to the membrane model. Using this approach we were able to reveal both the energetics and the diffusion coefficient of the lignin derivatives within the skin-like membrane model.

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Poster T2-14

Exploit propagation-induced distortion of the laser pulse to increase efficiency of high-harmonic generation

K Kovacs[1], V Tosa[1] and B Schütte[2]

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

[2] Max-Born-Institut, Max-Born-Strasse 2A, 12489 Berlin, Germany

E-mail: kkovacs@itim-cj.ro

Abstract. In a strongly overdriven configuration for high-order harmonic generation (HHG) we show the possibility to obtain an increased high-harmonic flux accompanied with the possibility to generate isolated attosecond pulse. The targeted spectral domains for the harmonic radiation in the XUV spectral domain are around 20 eV and 35 eV, respectively. Our main motivation is to facilitate the attosecond pump – attosecond probe experiments designed at Max Born Institut Berlin. We explain the mechanism of the driving pulse's blue shifting during propagation, investigate the influence of the initial chirp of the pulse, and we show the robustness of this configuration against carrier-to-envelope phase variation. The main reason for this is to relax the requirements for the experimental setup. The presented results have been obtained through simulations using a 3D non-adiabatic model for pulse propagation in Argon medium and HHG under high ionization conditions.

Poster T2-15

New material based on hydrogel and fruit wastes for pollutants removal from contaminated water

I Lung[1], M L Soran[1], O Opriș[1], A Stegarescu[1], AM Chiș[1], H Y Dasgan[2]

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

[2] Department of Horticulture, Faculty of Agriculture, University of Cukurova, Adana 01330, Turkey

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

Abstract. Pharmaceutical compounds from the aquatic ecosystems have become a concern in the last decade in the entire world because the pollutants can be accumulated and are considered as a potential risk to drinking water, human health and ecosystems. Due to the fact that pharmaceuticals compounds are not completely removed by conventional wastewater treatment plants, the adsorption technique using a suitable adsorbent could be a good option. For that reason, the selection of adsorbent is the most important point of view for successful adsorption process development, for its efficiency and operation. Adsorption using waste biomass materials is preferred to chemical synthesized adsorbents due to their low cost, simplicity, biodegradability and environmental friendly properties. Fruit wastes were investigated for pollutants removal and the hydrogels have applications in water purification due to excellent absorptive behavior.

The aim of this study was the preparation, characterization, and testing of a new material based on hydrogel and fruit wastes for paracetamol removal from contaminated water.

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Poster T2-16

Disrupting the aggregation propensity of cataract-associated P23T γD-crystallin by vitamin C

E Matei[1], A Filip[2], B Cozar[1], CG Floare[1], A Pîrnau[1], M Mic[1], A M Gronenborn[3]

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

[2] Enzymology and Applied Biocatalysis Research Centre, Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, Arany János Str. 11, 400028 Cluj-Napoca, Romania

[3] Department of Structural Biology, University of Pittsburgh, School of Medicine Pittsburgh, PA 15260, USA

E-mail: elena.matei@itim-cj.ro

Abstract. Cataract is a progressive loss of eye lens transparency, as a result of age-related chemical modifications or due to congenital mutations in crystallins. A vital antioxidant in the aqueous humor, the vitamin C, has been suggested to hold potential for the prophylaxis of age-related cataract. However, the effect of vitamin C on congenital cataract has not yet been investigated. Here, we explored the aggregation inhibitory effect of vitamin C on the P23T human γD-crystallin mutant, associated with congenital cataract. The effect of vitamin C on the aggregation propensity of P23T human γD-crystallin was investigated by solution NMR, atomic force microscopy (AFM), and other biophysical techniques. We found that vitamin C is able to prevent and reverse P23T human γD-crystallin aggregation in a dose-dependent manner. In particular, NMR data suggest that the inhibitory effect of vitamin C on P23T human γD-crystallin phase-separation is probably mediated by interacting with aggregation prone regions. AFM images of P23T human γD-crystallin under native aggregating conditions revealed the appearance of amorphous aggregates, that disassemble into monomers in the presence of vitamin C. The current study highlights and confirms the possibility that vitamin C is able to dissolve crystallin aggregates, potentially slowing the onset or reversing cataract.

Poster T2-17

Determination of quaternary ammonium compounds by GC/MS methods

Z Moldovan

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

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

Abstract. Quaternary Ammonium Compounds (sometimes called 'quats' or 'QACs') are a category of chemicals with a variety of uses, including controlling bacteria, viruses, and other germs on surfaces. In this paper will be discussed two categories of the QACs with general structure $[R_1R_2R_3R_4N]^+Cl^-$. One category is the Dialkyl Dimethyl Ammonium Chloride (DDAC) group which contains three similar chemicals, corresponding to alkyl group $[C_8]_2$, $[C_8,C_{10}]$ and $[C_{10}]_2$ respectively. Another category is the Alkyl Dimethyl Benzyl Ammonium Chloride (ADBAC) group. This group contains also three similar chemicals corresponding to alkyl group C_{12}, C_{14} and C_{16} respectively.

At the high temperature Quaternary Ammonium Compounds are eliminating R^+Cl^- resulting the Alkyl amines of general formula $R_1R_2R_3N$, three compounds from DDAC and six from ADBAC group. The paper describes the mass spectra of all nine compounds and the determination of initial QACs concentration using GC/MS analytical system based on mass spectrum and elution time.

Poster T2-18

Hidden Ingredients? Pesticide residue risk in frozen fruits and vegetables and fresh potatoes on the Romanian market

Cs Molnár[1,2], F D Covaciu[1], V Floare-Avram[1]

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

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

E-mail: csilla.molnar@itim-cj.ro

Abstract. The aim of this study was to assess potential health risks related to pesticide residues found in frozen fruits, vegetables, and potatoes available on the Romanian market. Risk levels were evaluated based on estimated daily intake (EDI), hazard quotient (HQ), and hazard index (HI). In the case of frozen produce, residues were identified in 48.5% of the analysed samples, with a few exceeding the EU maximum residue limits (MRLs)—specifically in spinach, peas, and carrots. Even so, all HQ and HI values remained below 1, suggesting no immediate risk to consumers. For potatoes, the situation was more concerning: out of 50 samples, 14 (28%) had HQ values above 1, mainly due to high levels of propiconazole and imazalil. HI values were above 1 in 16 samples (32%), including both Romanian-grown (9) and imported (7) potatoes, indicating a possible cumulative risk from multiple pesticide residues. These findings underline the need for regular monitoring and stricter control measures.

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Poster T2-19

Computational investigation of chirality-dependent azo coupling on Au(111) surfaces via DFT and STM simulations

C Morari, T Murariu, C Tripon and L Buimaga-Iarinca

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

E-mail: cristian.morari@itim-cj.ro

Abstract. We present a density functional theory (DFT) study on the role of porphyrin chirality in on-surface azo coupling reactions of Pt-porphyrin derivatives on Au(111). Using the SIESTA code with GGA-PBE exchange-correlation and Grimme D2 dispersion corrections, we modeled both homochiral and bichiral self-assembled structures, analyzing their stability, interaction with the surface, and reactivity. Systems were confined in periodic supercells with a vacuum buffer, ensuring decoupling between periodic images. Simulated STM images, based on the Tersoff-Hamann approximation, were generated from the local density of states in the relevant energy window, reproducing key experimental features. Our findings indicate that steric hindrance and chirality-induced molecular arrangements significantly impact the reaction yield by affecting the accessibility and alignment of reactive sites. This computational analysis provides mechanistic insight into the structure–reactivity relationship in surface-confined molecular systems and guides the design of efficient on-surface synthesis strategies.

Poster T2-20

Ultra-sensitive detection of astaxanthin by SERRS on AgFoN substrate

F Nekvapil[1], I Cârdan[1,2], D Cuibus[1], C Farcău[1]

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

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

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

Abstract. Astaxanthin is one of the most potent natural antioxidants, with great interest from pharma and nutraceuticals industries, as well as spectroscopy field. As with most natural compounds, research of astaxanthin encounters situations with low concentrations of the compound. In this study we explored the potential of SERS for quantification of ultra-low astaxanthin concentrations in a cost-effective manner. The mainstream method for astaxanthin quantification is HPLC coupled with UV-Vis absorption. Here, we used a broad-portable Raman spectrometer with acceptable cost-to-performance rate, deployable in biochemical labs. Our measurements and coupled with regression analysis show that SERRS using a substrate consisting of silica microspheres covered with Ag film and excited with 532 nm laser line enables astaxanthin quantification below the limits of mainstream methods. Supplementary measurements methods, such as Resonance Raman and UV-Vis absorption perform in astaxanthin range from 1.29 to 83.78 µM, while our SERRS method shows linear relationship of astaxanthin signal to its concentration in the range from 0.55 µM to 18.41 nM (0.33 to 0.01 µg ml^{-1}). We did not record any astaxanthin signal below the latter concentration. Our findings will be especially useful in biochemical studies of astaxanthin and its processing in pharmaceutical industry.

Poster T2-21

Polarization transfer efficiency in solid state NMR at spinning frequencies up to 150 kHz

A Simion[1,2], T Franks[3], S P Brown[3] and C Filip[1]

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

[2] Faculty of Physics, Babes-Bolyai University, 400084 Cluj-Napoca, Romania

[3] Department of Physics, University of Warwick, CV47AL Coventry, UK

E-mail: andrea.simion@itim-cj.ro

Abstract. Polarization transfer is central to many solid-state NMR experiments, yet achieving uniform signal enhancement remains challenging, especially under high MAS rates (>60 kHz) and strong magnetic fields (>28 T), where standard and double cross-polarization (CP) schemes often suffer. Key factors affecting transfer efficiency include dipolar coupling strength, RF field inhomogeneity, chemical shift dispersion, and molecular motion. However, a systematic evaluation of these effects under ultra-fast MAS conditions (>100 kHz) is still lacking.

In this work, we focus on the role of RF field inhomogeneity in polarization transfer efficiency using the standard CP sequence at MAS frequencies up to 150 kHz. Experiments were performed on uniformly ^{13}C-^{15}N-labeled glycine, with rotors filled in two ways to assess its influence. A loss in the signal up to 60% at 20 kHz MAS was observed, increasing to 90% at 150 kHz MAS due to RF inhomogeneity. We also explored polarization transfer via J-couplings using INEPT experiments. Remarkably, J-coupling-based transfer was achieved even at 150 kHz MAS. Finally, we compared results from a 0.5 mm homemade probe (high RF inhomogeneity) and a 1.3 mm Bruker probe (greater RF stability), highlighting their optimal conditions and performance differences.

Poster T2-22

Hyaluronic Acid as Biocompatible and Biodegradable Polymer Matrix for Ear, Nose and Throat Reconstructive Materials: In Vivo study

P Snetkov[1], M Naumenko[2], R Shaikenov[1], P Serbun[1], S Zhuravskii[2], S Morozkina[1]

[1] Institute of Advanced Data Transfer Systems, ITMO University, Kronverkskiy Pr., 49, bldg. A 197101 Saint Petersburg, Russia

[2] Experimental Pathomorphology Research Group, Almazov National Medical Research Center of the Ministry of Health of the Russian Federation, Akkuratova str. 2, 197341 Saint Petersburg, Russia

E-mail: ppsnetkov@itmo.ru

Abstract. Tympanic membrane perforation is one of the most difficult clinical problems at ENT (Ear, Nose and Throat) surgery, which can be caused by various reasons, including mechanical trauma, infection, or pressure changes, leading to hearing disability or complete hearing loss. Traditional surgical implants based on autologous tissues and synthetic materials have limitations: transplants cause pain, the synthetic transplants are not always biocompatible. Biopolymers are represent the preferable materials for such reconstructive purposes. In this study, the polymer films based on hyaluronic acid were developed as polymer matrix for reconstructive materials. Biocompatibility and biodegradability were evaluated on Wistar rats during a month using histological analysis. The *in vivo* experiment demonstrates the absence of acute toxicity, septic or allergic inflammation, and gross deforming scarring of surrounding tissues. At the end of the experiment, all samples are characterized by mild infiltration by actively phagocytic macrophages. Results obtained confirm biodegradability and biocompatibility of the films based on hyaluronic acid, and the possibility of its use as polymer matrixes for reconstructive surgery. However, additional techniques, such as cross-linking, should be used for the swelling limitation and the extending of the degradation time. This research was funded by the Russian Science Foundation, project number 25-73-20141.

Poster T2-23

Antifungal effects of *Rheum Rhabarbarum* extracts obtained by sonication

M L Soran[1], I Lung[1], O Opriș[1], S Jalbă[2], A Stegarescu[1], S Pintea[1], V Todiraș[2]

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

[2] Institute of Genetics, Physiology and Plant Protection, USM, Chișinău, Republic of Moldova

E-mail: loredana.soran@itim-cj.ro

Abstract. In the world, pathogens and pests, can reduce crop yields by up to 30%. In special conditions this loss can reach up to 80%. Chemical pesticides remain the first choice for crop protection in the world but the long-term and inappropriate use of chemical pesticides has resulted in more serious problems, (e.g pesticide residues in foods and soils, contamination of groundwater, rapid development of pesticide resistance, and other side effects). All these problems can destroyed the healthy community structure of agro-ecosystems with huge risks for humans. Natural products have been considered an important alternative strategy for sustainable pest management in agriculture. Rhubarb (*Rheum Rhabarbarum,* family Polygonaceae) is a perennial herbaceous plant widely sought for their rich nutraceutical values, presents a wide range of pharmacological activities because is rich in flavonoids, stilbenes, and anthraquinones, making it a valuable reservoir of phenolic antioxidants.

This study was conducted to screen this genotypes of Rhubarb for their phytochemical and antioxidant activity and parameters optimization for the sonication extraction method, in order to test their antifungal properties for natural crop protection.

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Poster T2-24

Tracking protein denaturation on gold nanoparticle surfaces: Insights into nano–bio interactions

C Rusu, D Stoia, A Holca, M Focsan

Biomolecular Physics Department, Faculty of Physics, Babes-Bolyai University,1 M. Kogalniceanu Street, 400084, Cluj-Napoca, Romania

Nanobiophotonics and Laser Microspectroscopy Center, Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, 42 Treboniu Laurian Street, 400271, Cluj-Napoca, Romania

E-mail: catalina.rusu@stud.ubbcluj.ro

Abstract. Gold nanoparticles (AuNPs) are well-known for their chemical stability, biocompatibility, and functional versatility, making them extremely valuable for biomedical research. Besides that, it is important to understand the behavior of nano-bio interfaces, especially how protein coronas behave on their surfaces under different conditions, in order to be efficiently integrated into therapeutic and diagnostic systems. This study investigates the structural evolution of bovine serum albumin (BSA) adsorbed on AuNPs surfaces under varying concentration and temperature conditions. The characterization is performed optically *via* UV-Vis-NIR extinction spectroscopy, Dynamic Light Scattering and Zeta Potential measurements, and morphologically by Transmission Electron Microscopy. Moreover, the behavior of the BSA protein corona was further analyzed using advanced spectroscopic methods such as fluorescence emission and Circular Dichroism, in order to assess its thermal stability and to study its secondary structure when adsorbed on AuNPs. Moreover, the samples were irradiated using a 532 nm laser to investigate their photothermal activity, and the resulting temperature increase was monitored using a thermal imaging camera. Overall, the results show that protein-functionalized nanoparticles are stable and may be used in target medication delivery in the future.

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Poster T2-25

Application of Fourier Transform Infrared Spectroscopy for evaluating the quality of different triticale varieties from the Republic of Moldova

A Ghendov-Mosanu[1], F Ursachi[2], I Rumeus[1,3], S Paiu[1], G G Codină[2] and R Sturza[1]

[1] Technical University of Moldova, 9/9 Studentilor St., MD-2045 Chisinau, Moldova

[2] "Stefan cel Mare" University, 720229 Suceava, Romania

[3] Cahul State University "Bogdan Petriceicu Hasdeu", 1 Independence Square, MD-3909 Cahul, Moldova

E-mail: aliona.mosanu@tpa.utm.md

Abstract. The aim of this study was to analyse the spectra of different triticale varieties from the Republic of Moldova obtained by FT-IR. For this purpose, seven wholemeal flours derived from triticale varieties Ingen 33, Ingen 35, Ingen 93, Ingen 54, Ingen 40, Fănica and Costel were analysed to evaluate the quality parameters of triticale grains by Fourier Transform Infrared Spectroscopy (FT-IR) using a Nicolet iS-20 spectrophotometer (Thermo Scientific, Karlsruhe, Dieselstraβe, Germany) in attenuated total reflectance mode. Several peaks were observed in the spectral range (4000-800 cm^{-1}), which correspond to compounds in triticale flour. FT-IR spectra obtained for the evaluated samples showed a similar spectral pattern for each of the triticale varieties, indicating similarity in terms of chemical composition. Thus, the spectral region 4000-2500 cm^{-1} corresponded to C-H stretching vibrations being considered for organic compounds, sugars, and starches; the spectral region 2500-2000 cm^{-1} corresponded to C=C and N-H or O-H stretching vibrations; and the spectral region 2000-1500 cm^{-1} corresponded to C=O stretching (carbonyl groups) or N-H bending vibrations. Peaks were also observed in the regions 800-1450 cm^{-1} (fingerprint region), which is highly specific to different types of chemical bonds and is used for identifying molecular structures. Different bending vibrations from bonds like C-H, C-C, and C-O stretching vibrations were presented in the spectral region 1000-800 cm^{-1}. According to the chemical data obtained, all triticale varieties may be used for breadmaking.

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Poster T2-26

Gold nanourchins for bionanosensoristics: a microfluidic approach

A S Tatar[1], I Brezestean[1], D Marconi[1], A Colnita[1] and S Boca[1,2]

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

[2] Interdisciplinary Research Institute in Bio-Nano-Sciences, Babes-Bolyai University, 400271 Cluj-Napoca, Romania

E-mail: andra.tatar@itim-cj.ro

Abstract. Anisotropic metal nanoparticles exhibit appealing optical properties, attributed to the intense electromagnetic fields concentrated at their geometric inflection points. Among these, gold nanourchins (GNUs) stand out due to their numerous sharp tips and indentations capable of high levels of signal enhancement through Surface Enhanced Raman Scattering (SERS). Furthermore, the gold surface can be bio-functionalized with recognition molecules such as aptamers for binding of target disease biomarkers. However, a limitation of anisotropic particles is the low reproducibility of synthesis. Sensor applications demand consistent and accurate detection and quantification of target analytes. Adopting a microfluidic approach for the synthesis of gold nanourchins is a crucial advancement, as it ensures controlled flow and uniform reactant mixing, resulting in a significantly more monodisperse nanoparticle yield. The particles were biofunctionalized with anti-Tau aptamers for detecting the Alzheimer's disease biomarker protein Tau, and spectroscopically and morphologically characterized. SERS measurements identified bands with strong correlation to the analyte concentration, showing the proposed systems' potential for bionanosensoristics. This system offers advantages such as minimal sample requirements, rapid detection, and potential for point-of-care applications. Future work will focus on optimizing the detection sensitivity and expanding the system's capabilities for other relevant biomarkers.

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Poster T2-27

Surface vs bulk sensitivity of plasmon resonances in nanoparticle ensembles

I Toth and C Farcau

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

E-mail: istvan.toth@itim-cj.ro, cfarcau@itim-cj.ro

Abstract. Localized surface plasmon resonances represent the collective motion of bulk conduction electrons in metallic nanoparticles induced by incoming electromagnetic radiation. The sensitivity of these resonances to their environment sets the basis for developing practical applications in the field of chemo- and biosensing. In this study we comparatively investigate by Finite-Difference Time-Domain (FDTD) simulations the surface vs bulk sensitivity of ensembles of irradiated nanoparticles of different shapes. The change in the refractive index of the environment was obtained by changing the medium surrounding the ensemble. Locally the refractive index is changed by considering layers of dielectric materials on the surface of the metallic nanoparticles. We also compare single to coupled nanoparticles and show how the sensitivity is affected by interparticle gaps.

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Poster T2-28

Assessment of shape- and dose-dependent hepatotoxicity induced by gold nanoparticles in an in vivo model

Sz Toth[1,3,4], A Vădan[1,3,4], A D Stoica[2,3,4] and S Boca[2,5]

[1] Doctoral School of Integrative Biology, Babes-Bolyai University, Cluj-Napoca, 400015, Romania

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

[3] Departament of Molecular Biology and Biotechnology, Faculty of Biology and Geology, Babes-Bolyai University, Cluj-Napoca, 400015, Romania

[4] Centre 3B, Babes-Bolyai University, Cluj-Napoca, 400015, Romania

[5] Interdisciplinary Research Institute in Bio-Nano-Sciences, Babes-Bolyai University, Cluj-Napoca, 400271, Romania

E-mail: anca.stoica@ubbcluj.ro

Abstract. Gold nanoparticles (AuNPs) have become a promising tool in targeted cancer therapy as drug delivery systems, due to their small size, high surface-to-volume ratio and capability to be chemically conjugated with anticancer drugs. Besides drug delivery, AuNPs can also trigger the production of reactive oxygen species (ROS) and ferroptosis, leading to cytotoxic effects. This study assessed the *in vivo* hepatotoxicity of two AuNP shapes (quasi-spherical and bone-like) in female Wistar rats. Animals received intravenous treatment of one, two or four doses of each AuNP types over 14 days. Oxidative stress parameters and hepatic enzyme activity were measured to evaluate liver function. An enhanced concentration of plasma malondialdehyde and reduced levels of glutathione were detected in groups treated with two or four NPs injections. Alanine aminotransferase (ALAT) activity was elevated in both multi-dose groups, while the activity of aspartate aminotransferase (ASAT) was increased in the subjects receiving four doses of each NPs type. These findings suggested a dose-dependent hepatotoxicity associated with AuNPs of two distinct shapes, consisting in the disruption of hepatocyte membrane integrity. Based on the results obtained in the presented in vivo model, we infer that an adjustment of the AuNPs morphological characteristics would contribute to the alleviation of the induced toxicological effects.

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Poster T2-29

Poly (Lactic-*co*-Glycolic Acid) nanoparticles encapsulating IR-783 fluorophore for NIR imaging and photothermal therapy

M Tudor[1,2], D Dămoc[1], R Borlan[2], M Muntean[3], O Soriţău[4], D Maniu[1,2], M Focşan[1,2]

[1] Biomolecular Physics Department, Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Cluj, Romania
[2] Nanobiophotonics and Laser Microspectroscopy Centre, Interdisciplinary Research Institute in Bio-Nano-Sciences, Babeș-Bolyai University, Cluj-Napoca, Cluj, Romania
[3] Department of Cell and Molecular Biology, Faculty of Medicine, Iuliu Hatieganu University of Medicine and Pharmacy, Cluj-Napoca, Cluj, Romania
[4] Department of Radiobiology and Tumor Biology, Oncology Institute Prof. Dr. Ion Chiricuta, Cluj-Napoca, Cluj, Romania

E-mail: madalina.tudor@stud.ubbcluj.ro

Abstract. Poly(lactic-co-glycolic acid) (PLGA), an FDA-approved biodegradable polymer, is widely utilized in the development of long-acting drug delivery systems for cancer therapy. In this study, we developed PLGA nanoparticles encapsulating the near-infrared (NIR) fluorophore IR-783 (PLGA@IR783 NPs) for potential preclinical applications in cancer theranostics. Nanoparticles were synthesized via a single emulsion method, yielding a mean hydrodynamic diameter of 229.2 ± 1.1 nm with a low polydispersity index (PDI = 0.09 ± 0.01) and a zeta potential of -29.0 ± 1.0 mV, indicating good colloidal stability. Transmission electron microscopy confirmed spherical morphology and uniform size distribution. Optical analysis revealed a fluorescence emission peak at 801 nm, while photothermal performance under 808 nm laser irradiation was confirmed using an infrared camera. *In vitro* studies on OVCAR3 (ovarian carcinoma) and THP-1 (monocytic leukemia) cell lines demonstrated high biocompatibility and efficient cellular uptake, as visualized through fluorescence imaging. These results suggest that PLGA@IR783 NPs represent a promising approach for integrated imaging and photothermal therapy, combining favorable physicochemical characteristics with effective biological performance.

Poster T2-30

The energetics of short Trp- and Arg-rich antimicrobial peptides at lipid-water interfaces

I Turcu[1], G Necula[2] and L Janosi[3]

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

[2] Department of Computational Physics and Information Technologies, Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, 077125 Magurele, Romania

E-mail: ioan.turcu@itim-cj.ro

Abstract. Our work is focused on the accumulation of short cationic antimicrobial peptides (AMPs) at the water-lipid bilayer interface. Combining molecular dynamics simulations and statistical physics we obtained the AMP partition difference between the aqueous bulk and the lipid-water interface region. The main goal is to unravel the energetics of molecular interaction of a specific AMP with different membrane models. We investigated a short Trp- and Arg-rich AMP, interacting with a pure phosphatidylcholine (PC) and an 85:15 mixture of PC with phosphatidylglycerol (PG) lipids as models for mammalian and bacterial membranes, respectively. Potential of mean force profiles were used to calculate binding free energies of the short AMPs to the lipid bilayer models.The obtained Gibbs free energies revealed significant differences of the AMP partitioning at the interface for the two bilayers, suggesting a qualitatively different insertion of cationic AMP into the mammalian and bacterial membrane models.Our results provide novel insights into the energetics of short Trp- and Arg-rich cationic peptides located at the lipid-water interface.

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SECTION T3

Green Energy and Innovative Technologies

Oral T3-1

Enhancing the supercapacitor performance by using W-doped SnO_2 electrode material

A U Ammar[1], A Rostas[1], D Toloman[1], A Popa[1], M Stefan[1], E Erdem[1,2]

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

[2] Faculty of Engineering and Natural Sciences, Sabanci University, Tuzla, Istanbul, 34956, Turkey

E-mail: ameen.ammar@itim-cj.ro

Abstract. This study explores the potential of SnO_2-based materials for high-performance supercapacitor applications by incorporating W^{5+} and W^{6+} as dopant ions. To investigate the influence of tungsten doping on the electrochemical behavior of SnO_2, the materials were extensively characterized and tested as electrode materials. Morphological and structural analysis was carried out using SEM, TEM, XRD, Raman spectroscopy, and XPS. The impact of tungsten doping on the defect structure and oxidation states was examined through electron paramagnetic resonance (EPR) and photoluminescence (PL) spectroscopy. Electrochemical performance was evaluated for both undoped and W-doped SnO_2 electrodes in all-in-one symmetrical supercapacitor configurations. The W-doped SnO_2 demonstrated a notable performance improvement, achieving a maximum specific capacitance of 268 F/g, along with enhanced energy and power densities of 36.8 Wh/kg and 2650 W/kg, respectively.

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Oral T3-2

Cold plasma-assisted oxidation of glycerin

M Coros, C Tudoran and G Blanita

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

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

Abstract. Glycerin is a by-product of biodiesel production that can be transformed into high-value compounds. However, its conversion through selective oxidation remains challenging. Due to its unique properties, plasma can potentially facilitate the oxidation of the two types of hydroxyl groups found in glycerin.

Cold plasma applied in solution is an innovative and environmentally friendly technique that simplifies the synthesis process, reduces reagent consumption, shortens reaction times, and allows for ambient processing conditions. This study investigates the oxidation of glycerin using cold plasma-assisted oxidation. A cold plasma reactor was conceived, designed, and constructed specifically for this purpose.

Oral T3-3

Visualizing Electromagnetic Fields: A robotic approach to antenna radiation mapping

R Gutt[1], V Surducan[1], O R Bruj[1], I A Nadăș[1], R Nelega[1,2], G Kovács[1,2] and A D Oprea[1]

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

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

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

Abstract. This presentation introduces a system developed at INCDTIM for measuring, visualizing, and analyzing the far-field radiation pattern of antennas. Based on the results gained from a previous research project, the system integrates a robotic arm for spatial scanning with a custom software application for control, data acquisition, and 3D visualization. Central to the system is an in-house developed antenna array detector consisting of 8 broadband microwave sensors, operating in the 500 MHz – 3 GHz range. The system employs an RGB-based visualization technique, mapping microwave power density to eight color-coded thresholds, enabling intuitive interpretation of electromagnetic field distributions. Experimental results demonstrate the system's ability to assess radiation patterns from radar modules and mobile phone signals, including web traffic emissions. This work simplifies the evaluation of electromagnetic fields, offering a practical and accessible tool for antenna diagnostics with applications in research, education, and RF safety analysis.

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Oral T3-4

Dielectric properties of layered double hydroxides (ldhs) and applications for nano energy generators

P G Medaglia[1], C. Falconi[2], N J Calavita[1], C Leonardi[1], R Pezzilli[1], G Prestopino[1], D Citernino[1], F Delle Fave[1] and M Froio[1]

[1] Department of Industrial Engineering, University of Rome "Tor Vergata", Rome, I-00133, Italy

[2] Department of Electronic Engineering, University of Rome "Tor Vergata", Rome, I-00133, Italy

E-mail: medaglia@uniroma2.it

Abstract. Layered Double Hydroxides (LDHs), are a large family of 2D layered nanostructured materials, covering a wide range of fields of interest, including sensing, drug delivery, flame retardants systems, energy storage, catalysis and many others. We report on novel possible applications of these nanostructured dielectric materials as nano energy generators, by exploiting the energy harvesting obtainable from waste ambient thermal and mechanical fluctuations. In particular, we show first observations of pyroelectricity as a consequence of time-dependent temperature variations, and tribo- piezo- electricity from mechanical stimuli, observed in arrays of (Mg,Al)/LDH and (Zn,Al)/LDH nanoplatelets, synthesized on different substrates.

Oral T3-5

Non-destructive investigation of microfluidic channels in fused silica by optical coherent tomography and microscopy

N Tosa[1], R Martínez Vázquez[2,3] and V Tosa[1]

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

[2] Italian National Research Council, Institute for Photonics and Nanotechnologies (CNR-IFN), Piazza L. da Vinci 32, 20133 Milan, Italy

[3]Department of Physics, Polytechnic University of Milan, Piazza L. da Vinci 32, 20133 Milan, Italy

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

Abstract. The aim of this work is to investigate the morphology of femtosecond laser micromachined microfluidic channels in fused silica in a non-invasive and non-destructive manner using optical microscopy as well as spectral domain optical coherent tomography (SD-OCT) in 1200-1400 nm domain. Multiple image alignment optical images present channels with 7.73 cm length, with 100 µm diameter inlets, located at a distance of 1100 µm from each other. The lateral XZ and YZ 2D images show a relatively constant 147.5 µm diameter of the ablated channel along its length except the first 500 microns from the entrance, where the diameter is around 116 µm. The 3D OCT images in volumetric mode show a continuous and well-defined micromachined channels, situated inside of the 1 mm thickness fused silica plate at 147 to 120 micrometers related to the upper surface. The advantage of the OCT technique is that the morphology of the channels can be analysed without any preconditioning of the sample or destroying it to have direct access inside of the channel. The support of this work by European Union’s Horizon 2020 Research and Innovation Programme under Grant Agreement No. 964588 (XPIC) and by ‘Nucleu’ Program, project code PN 23240102, is acknowledged.

Oral T3-6

The Romanian quantum communications network

L P Zarbo

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

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

Abstract The Romanian Quantum Communications Network (RoNaQCI has been a project spanning two years and six months. Its objective was to build the first quantum network infrastructure in Romania, and it has been within the scope of the larger European effort, EuroQCI, which aims to build the quantum internet, an online space, in which data transmissions are unconditionally secure, and quantum resources are available to all users. It will be presented the implementation of this project in Romania and the significance of its results, together with the main achievements of the project, outlining the role of our team at INCDTIM.

Poster T3-1

Experimental validation of a two-pole permanent magnet synchronous generator for small wind turbines

E Bruj, O Bruj, S Gergely and V Surducan

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

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

Abstract. Permanent magnet synchronous generators (PMSG) are widely used in small wind turbines due to their high efficiency and easy maintenance. Latest designs focus on direct-drives systems and different magnet arrangements. In order to increase the efficiency of the generator by enhancing the magnetic fields and reduce the energy losses, the permanent magnets in the rotor are placed in a Halbach arrangement. The PMSG under study has two poles and NdFeB magnets in the rotor to create a radial flux path. Numerical simulations are used to determine the total losses of the generator. Experimental measurements were conducted in order to validate the numerical analysis.

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Poster T3-2

Phase change materials for an effective thermal management system of Li-Ion batteries

O Bruj, M Zagrai, A Turza, T Radu and E Bruj

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

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

Abstract. Phase change materials (PCMs) have emerged as an innovative solution in thermal energy storage and thermal management systems (TMS) owing to their outstanding latent heat of fusion during the phase change process. This study is especially addressed to the battery TMS based on Organic PCMs for fast charging/discharging applications of lithium-ion batteries (LIBs). These fast processes generate excessive heat during operation, degrade battery performance, decrease the energy efficiency and reduce the lifespan and safety of batteries. Organic PCMs, exhibit desirable properties, including high latent heat capacity, good thermal characteristics, low cost, and ease of integration. The major challenge for the successful application of organic PCM is the low thermal conductivity which impacts the heat storage and release rates. PCM based Paraffin Wax (PW) has been designed by including expanded graphite (EG) as high thermal conductivity additive. Experiments focused on the effects of different heat treatment of expandable graphite involved over the fabrication process of EG, EG concentration, and compression mode on the thermal conductivity performance of PCM composites. Crystal and chemical structure of investigation samples were analysed by XRD and FTIR spectroscopy. The battery module created with prepared PCM composites were ample examined using charging/discharging experiments at different C-rates.

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Poster T3-3

Impact of renewable energy injection on transport infrastructure: a technical and systemic analysis

L A Dina[1], P M Mircea[2], I Marin[3] and I Iordache[1]

[1] National Institute for Research-Development and Testing in Electrical Engineering, Craiova, Romania.

[2] Electrical Eng., Energ. and Aerospace Department, University of Craiova, Craiova, Romania.

[3] Network Management Department, Energy Distribution, Oltenia, Craiova, Romania

E-mail: liviadina@icmet.ro

Abstract. The accelerated integration of renewable energy sources, particularly wind and solar power, into modern energy systems is an essential step towards decarbonisation and reducing dependence on fossil fuels. However, this transition also brings a number of significant challenges for power transmission networks and, especially, for distribution networks. Among the most relevant are natural variability and unpredictability of production, risks of overloading the existing infrastructure, the emergence of bidirectional power flows, and reduced network stability due to lack of systemic inertia. Furthermore, growing demands for real-time balancing of production and consumption involve investments in fast-response resources and efficient storage solutions. Last but not least, the geographical dispersion of renewable capacities requires an advanced digital infrastructure capable to ensure precise coordination and robust control of the energy flows. Benefiting from the institutional and technological expertise of National Institute for Research-Development and Testing in Electrical Engineering - ICMET Craiova, this work provides an overview of the impact of renewable energy generation on power transmission/distribution networks and explores applicable solutions for the sustainable and secure integration of these sources into the national energy system.

Poster T3-4

SnSe as a promising 2D material for thermoelectric devices

S Garabagiu, D Marconi, D Bogdan, G Borodi and V Surducan

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

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

Abstract. SnSe, with its simple, orthorhombic structure, is a *-p* type semiconductor with an optical band gap below 1eV. Recent findings have shown that polycrystalline SnSe can achieve a figure of merit (zT) of 3.1 at 783 K, exceeding the performance of its single-crystal (zT=2.6), previously known as “the best thermoelectric”. Nanostructuring is supposed to improve the thermoelectric properties of materials, by altering their structure at the nanoscale. In this work, highly oriented (040) SnSe thin films have been fabricated by Pulsed Laser Deposition (PLD) on quartz substrates. Both optical band-gaps and Seebeck coefficient measurements were similar with the values mentioned in the literature. Seebeck coefficient measurements were performed using a custom-built device patented by our institute. The results confirm the thermoelectric potential of these thin films. Future goals are to improve the performances of these films, and include them in miniaturized thermoelectric generators.

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Poster T3-5

TVZ-H as innovative catalyst used in degradation processes of polyolefin polymers

R C Gavrea[1], M Zagrai[1], R A Mereu[2] and S Burcă[2]

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

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

E-mail: silvia.burca@ubbcluj.ro

Abstract. Pyrolysis of plastic waste is considered one of the most feasible methods of its recycling, fuels obtained in the gas or liquid phase can greatly contribute to environmental conservation and intensification of the recovery of petroleum products. This study reports the synthesis of the volcanic tuff zeolite-based catalyst and the evaluation of the catalytic activity in the catalytic degradation process of high-density polyethylene (HDPE) and polypropylene (PP). The experiments were conducted in a batch reactor at atmospheric pressure, with a heating rate of 25 ° C/min up to a temperature of 500 °C and a mass ratio catalyst: polymer of 1:10. Higher conversion values were recorded for the catalytic degradation process, between 92% and 97% compared to the non-catalytic degradation process, between 81 and 90%. For TVZ-H catalyst, the degradation process begins at a lower temperature (220 -225 °C) than in the case of the non-catalytic process (248 - 250 °C). For the catalytic process, the major product was a liquid fraction, mostly distillate oil while in the case of thermal pyrolysis the main products were gases. The thermal behaviour and chemical composition of study samples were evaluated using Thermogravimetric analysis (TGA) and Fourier Transform Infrared (FTIR) spectroscopy.

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Poster T3-6

Real-time single-photon pulse counting with low-cost microcontrollers

T Murariu[1], L M Pioraș-Țimbolmas[1,2], C Tudoran[1], C Tripon[1], L Buimaga-Iarinca[1], L Zârbo[1], and C Morari[1]

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

[2] Faculty of Physics, Babeș-Bolyai University, 1 Kogâlniceanu, Cluj-Napoca, Cluj 400084, România

E-mail: teodora.murariu@itim-cj.ro

Abstract. The measurement process is a crucial element for the interpretation of results in quantum mechanics experiments. In this work, we designed and employed a microcontroller-based system for data acquisition in a down-conversion experiment aimed at detecting single-photon events. This setup enables us to investigate the impact of the detector's dead time and electronic acquisition delays on the measured data. By applying different time windows during single-photon data collection, we estimate the measurement errors as a function of the correlation between electronic delay and detector dead time. Our findings are supported by analysing particle counts, detection rates, statistical distributions, and the correlations between signal and idle photons.

Poster T3-7

Enhancing supercapacitor performance with tungsten-doped molybdenum disulfide

I Nesterovschi[1,3], A U Ammar[1], A Varadi[1,2], A Popa[1], M Stefan[1], S Macavei[1], E Erdem[1,4], A M Rostas[1] and D Toloman[1]
[1]National Institute for Research and Development of Isotopic and Molecular Technologies, Donat 67-103, Cluj-Napoca, 400293, Romania
[2]Doctoral School of Chemistry, Babes-Bolyai University, Cluj-Napoca, 400084, Romania
[3]Doctoral School of Physics, Babes-Bolyai University, Cluj-Napoca, 400084, Romania
[4]Faculty of Engineering and Natural Sciences, Sabanci University, Tuzla, Istanbul, 34956, Turkey

E-mail: ion.nesterovschi@itim-cj.ro

Abstract. Molybdenum disulfide (MoS_2) represents a promising material for supercapacitor applications due to its layered structure, large surface area, and high chemical stability, which altogether results in a robust electrochemical performance. However, its moderate electrical conductivity can limit its energy storage capacity. To solve this, MoS_2 was doped with tungsten (W) at varying concentrations (0.3–1%) to change its electronic structure and enhance charge transport. Electrochemical testing revealed that MoS_2 doped with 0.7% W achieved a remarkable specific capacitance of 480 F/g, compared to 150 F/g for the undoped sample. Additionally, the doped material exhibited a power density of 480 W/kg and an energy density of 67 Wh/kg - significantly surpassing the undoped sample (140 W/kg and 20 Wh/kg, respectively). A set of characterization techniques, including TEM, UV-Vis, Raman, IR, XRD, PL, and EPR, was used to correlate this performance with structural and electronic modifications, particularly the introduction of beneficial defects. These findings demonstrate the strong potential of W-doped MoS_2 as a high-performance electrode material for next-generation energy storage devices.

Poster T3-8

Development and performance evaluation of Dye-Sensitized Solar Cells: material optimization and photovoltaic characterization

A D Oprea, I Craciunescu, M Zagrai and V Rednic

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

E-mail: alexandru.oprea@itim-cj.ro

Abstract. Dye-Sensitized Solar Cells (DSSCs) represent a promising class of low-cost, environmentally friendly photovoltaic technologies capable of functioning under diffuse and low-light conditions. In this study, dye-sensitized solar cells (DSSC) were fabricated incorporating titanium dioxide (TiO_2) semiconductor layer deposited through a facile and environmental friendly method onto conductive indium tin oxide (ITO)-coated glass substrate. The photoanode was sensitized using an anthocyanin-based organic dye extracted from blueberry (Vaccinium spp.) fruits, selected for its natural abundance and eco-compatibility. The redox electrolyte comprised an iodide/triiodide (I^-/I_3^-) system, further modified with specific additives to enhance ionic conductivity and charge transport efficiency. A graphite-based counter electrode was employed, offering a low-cost and sustainable alternative to conventional platinum electrodes while maintaining adequate catalytic activity for electrolyte regeneration. Photovoltaic performance was evaluated using a lamp designed to emit across the full solar spectrum. Key parameters such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and overall power conversion efficiency (PCE) were measured and compared across different configurations.

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Poster T3-9

Energy management for an environmental monitoring system relying on solar power

M N Pop

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

E-mail: pop.mircea.n@protonmail.com

Abstract. The measurement of different parameters of the environment, in remote locations is often necessary for monitoring purposes. In case of remote locations, where power may not be permanently available, two bottlenecks emerge from the power management viewpoint of: i. data acquisition and storage and ii. data transmission and additional communication operations. An energy management sub- system for an environmental measurement system, provided with autonomous power is presented herein. The environmental measurement system uses on-board and external sensors in order to acquire environmental data (temperature, humidity, atmospheric pressure, vibration, position and air quality) and is meant to be powered exclusively from harvested solar energy. Acquired data is recorded to a local memory unit and can be sent on request. The environmental sensing system obtains energy from a solar panel and the harvested electrical energy is stored into a local Li-Ion battery. An energy management sub-system is meant to keep evidence of the stored, readily-available and consumed energy in order to maintain the accumulated energy above a safety level so that the system can continuously accomplish its main function, the gathering of environmental data. The energy management sub-system is able to i. measure the instantaneous power flow from the generator, to the battery and to the load, ii. to estimate the availability of stored energy and iii. to set the schedule-specific parameters of the environmental measurement system.

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Poster T3-10

Metallic nanocomposites as substitute for cement in the preparing of mortars

R Rada[1], A Nowakovski[3], B Dutka[3], R Chelcea[1], D L Manea[1], C Aciu[1], K Godyn[3], M Tram[3], S Rada[1, 2]

[1]Technical University of Cluj-Napoca, 28 Memorandumului, 400020 Cluj-Napoca, Romania

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

[3] Strata Mechanics Research Institute, Polish Academy of Sciences, 30-059 Krakow, Poland

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

Abstract. The applications of supplementary materials in cement - based materials have a significant attention nowadays due to the reduction of carbon emissions and the formation of hydration products. Nanocomposites containing construction and demolition waste such as iron, steel, lead and ash are expected to produce a sustainable construction material. In this paper the effect of incorporation of the nanocomposites as a replacement of Portland cement in mortar was studied. Composites based on a mix of four construction and demolition waste were added in the mortar considering the substitution of 2.5, 3, 5 and 10 % cement in the mortar mass. The structure and mechanical properties of the composite – mortar samples were investigated by analysis of X – ray diffraction (XRD), nuclear magnetic resonance (NMR) spectra and uniaxial tensile tests. For the mortars replacing with 3.5 and 5 % composites were observed an increasing trend in the values of the compressive strength comparatively with standard mortar. The observed enhancements in strength coupled with economic advantages stand new composites based on recycled metallic waste for the construction applications.

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Poster T3-11

Passive sampling for Cd determination in wastewaters using a new polymer inclusion membrane

M Senila, S B Angyus, L Senila and E Kovacs

INCDO-INOE Research Institute for Analytical Instrumentation, 67 Donath, 400293, Cluj-Napoca, Romania

E-mail: marin.senila@icia.ro

Abstract. Cadmium is classified as a priority hazardous element, even at low concentrations. Thus, highly sensitive analytical methodologies are essential for assessing environmental contamination and human exposure. In passive sampling technique the analyte migrates from the sampled medium to a collecting medium based on its free diffusion. This method offers several advantages over grab sampling, including the potential for analyte preconcentration and separation from complex matrices. Among the available tools for passive sampling, polymer inclusion membranes (PIMs) have been recently developed due to their numerous benefits. By utilizing PIMs, both extraction and back-extraction occur simultaneously, providing excellent selectivity. A PIM consists of an extractant encapsulated in a polymeric matrix that serves as a binding reagent for the analyte. The analyte is then back-extracted into a receiving solution. This work reports on the application of a new PIM prepared using poly(vinyl chloride) (PVC) as the base polymer, dioctyl phthalate (DOP) as the plasticizer, and Chelex-100 as the carrier. Extraction experiments were conducted using a Cd(II) solution at a concentration of 10 mg L−1 as the donor phase. The results demonstrated strong performance in the transport of Cd(II) ions, with approximately 92% of the analyte being extracted from the feed solution.

Poster T3-12

Restoration of the blurred image which is due to linear motion

F Toadere

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

E-mail: ftoadere@itim-cj.ro

Abstract. Linear motion restoration refers to the process of recovering a clear image from one that has been linearly blurred during picture acquiring. To address this common problem in photography an algorithm which recovers the images taken during liner movment image acquiring, is presented. Thus, the point spread function (PSF) of the motion is computed by employing a cepstrum which compute the angle and length of the motion which blurs the image. Then PSF finte dimesion is put inside the larger dimensions of a zero matrix having the size of the blurred image. Finally. The movement image is restored via deconvolution of motion PSF from the blured image. Demostrative images are presented in order to show the fulfiling of the restoration task.

Poster T3-13

Generation of attosecond pulses in guided structures by mid-IR femtosecond pulses

V Tosa, A M M Gherman, I F Toth, K Kovacs

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

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

Abstract. Attosecond pulses, either isolated or in trains, are generated in the interaction of high intensity femtosecond pulses with condensed or gas media. For hosting the gas media either static cells, gas jets expanded in vacuum or hollow core waveguides (HCW) are used. We analyse here this last case because it has many advantages which can enhance the generation efficiency. On one hand one can use higher gas densities over long distances and impose a specific variation of this density along the HCW, which can be linked to the laser intensity variation, inducing in this way a quasi-phase-matching regime of generation. On the other hand the laser intensity can be maintained along the guide at higher intensities while the propagation in un-guided structures the plasma defocusing produce a faster decrease of the field strength. We will present results obtained via numerical modelling in Ar, Ne, and He irradiated with mid-IR femtosecond pulses in geometries relevant for experiments performed in the framework of the H2020 X-PIC project.

Poster T3-14

Glass and glass-ceramics materials for high-temperature sensible energy storage

M Zagrai[1], A Turza[1], O R Nemethi[2], C C Vagner[2] and R A Mereu[2]

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

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

E-mail: raluca.mereu@ubbcluj.ro

Abstract. Thermal energy storage (TES) systems have emerged as one of the most promising technologies for efficient collection and utilization of solar energy to address energy demands and environmental concerns. TES systems typically consist of a storage medium, a container, and input/output devices and storage medium is the core elements of the systems responsible for absorbing and releasing thermal energy. Thermophysical, chemical, optical, environmental, and economic characteristics are crucial for cost-effective TES systems, especially in applications such as concentrated solar power. Glass materials have been explored in different technology applications and are attractive candidates for TES systems operating at elevated temperatures. The ability to operate at high temperatures will significantly increase the efficiency of heat-to-electricity conversion. In addition, its chemical stability allows for long-term heat storage, while its low cost and recyclability make it a cost-effective and environmentally sustainable option. The present work focuses on the effect of chemical composition and heat treatment temperature on the redox state of iron in Na_2O-CaO-SiO_2 glass and glass-ceramics system to evaluate its potential as a TES material. The chemical structure, thermal behaviour, and optical characteristics of study samples were evaluated using X-ray Diffraction, Thermogravimetric analysis (TGA), Fourier Transform Infrared (FTIR) and Ultraviolet-visible (UV-Vis) spectroscopy.

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SECTION T4

Nanostructured and Hybrid Materials

Oral T4-1

Differences and similarities in the behavior of Mo- and Sn-containing composite supported Pt electrocatalysts

I Borbáth[1], Z Pászti[1], C Silva[1], G Sáfrán[2] and A Tompos[1]

[1] Institute of Materials and Environmental Chemistry, HUN-REN Research Centre for Natural Sciences, Magyar Tudósok körútja 2, H-1117 Budapest, Hungary

[2] Institute for Technical Physics and Materials Science, HUN-REN Centre for Energy Research, Konkoly-Thege Miklós út 29-33, H-1121, Budapest, Hungary

E-mail: borbath.irina@ttk.hu

Abstract. Oxophilic metal (Mo, Sn)-doped TiO_2-carbon composites were identified as promising multifunctional supports for Pt electrocatalysts, in which the oxide component enhances resistance against corrosion and strong metal-support interactions at the Pt-oxide boundary ensure high stability for the Pt nanoparticles. Both the Mo- and Sn-containing composite supports were prepared by the same ideal structure in mind (i.e., good coverage of oxide component over the high surface area carbon). The structural, compositional and morphological differences between the samples prepared using $Ti_{(1-x)}M_xO_2$-C (M: Mo, Sn; x: 0.1-0.2) composites on the electrocatalytic behavior and stability of the synthesized Pt catalysts were investigated by spectroscopic, microscopic and electrochemical techniques. Elemental mapping evidenced close association between Pt and dopant (M: Mo, Sn) for both catalyst systems, which has a decisive influence on the electrocatalytic activity. Reductive pre-treatment results in the migration of Mo species to the Pt surface without overcoating the Pt sites, whereas in the case of tin it leads to the Sn-Pt alloy formation.

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Oral T4-2

Innovative magnetic nanocluster-coated sawdust for eco-friendly oil cleanup in water systems

I Craciunescu, G M Ispas, S C Tripon, R P Turcu

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

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

Abstract. We present an innovative system for oil removal from wastewater based on a bio-derived magnetic composite, developed from recycled sawdust and functionalized with advanced nanocluster technology. The composite consists of magnetic clusters coated with silicon dioxide (SiO_2) to ensure structural stability, followed by surface modification with 3-Trimethoxysilylpropyl methacrylate (TPM) to achieve superhydrophobic and oleophilic properties. In contrast to conventional magnetic systems using isolated magnetite nanoparticles, our approach uses stabilized magnetic clusters, which exhibit superior responsiveness to external magnetic fields and minimize aggregation. The magnetic composite is adsorbed onto the sawdust substrate, enabling rapid, selective, and efficient separation of oils from water. The use of recycled sawdust as a low-cost, sustainable support material enhances both the economic and environmental value of the system. Adsorption tests demonstrated high oil recovery efficiencies ranging from 93% to 97% across various oil types, highlighting the material's robustness and real-world applicability for environmental remediation. This work demonstrates the potential of combining green materials with nanotechnology for scalable, cost-effective solutions to water pollution.

Oral T4-3

Novel, biodegradable magnetic nanocomplexes aimed at magnetic resonance imaging

C Feoli[1,2], J Adam[2], A Brunetti[2], P Cicatiello[3], S Clemente[4], S Cocozza[2], R Pacelli[1,2], M Quarantelli[5], G Rusciano[6], A Sasso[6], R Schiano[4], M Singh[7], M Valadan[8], I Craciunescu[9], G Ispas[9], R Turcu[9], P Sandra[10] and R Kurapati[10], C Altucci[2]

[1] A.O.U University Hospital Federico II, 80131, Naples, Italy
[2] Department of Advanced Biomedical Sciences, University of Naples Federico II, Naples, Italy
[3] Department of Chemical Sciences, University of Naples "Federico II", Naples, Italy
[4] Unit of Medical Physics and Radioprotection, A.O.U Policlinico Federico II, 80131, Naples, Italy
[5] Biostructure and Bioimaging Institute, National Research Council, Via T. De Amicis 95, 80145 Naples, Italy.
[6] Department of Physics "Ettore Pancini", University of Naples "Federico II", Naples, Italy.
[7] Department of Physics, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133, Milano, Italy.
[8] CNR-SPIN (SuPerconducting and other INnovative materials and devices institute), Compl. Universitario di Monte S. Angelo, Via Cintia, 80126, Napoli, Italy
[9] National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
[10] School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, Maruthamala P.O., Vithura, Thiruvananthapuram, Kerala 695551, India

E-mail: chiara.feoli@unina.it

Abstract. Iron oxide (Fe_3O_4) and Manganese-based nanoparticles (NPs) have been extensively studied as T1 and T2 contrast agents (CAs) in magnetic resonance imaging (MRI). Despite the Gadolinium-based CAs are considered the gold standard for T1-weighted images in the clinical application, these molecules are not biodegradable. This study aims to combine the properties of MnO_2 and Fe_3O_4 nanoparticles and design, fabricate, and characterize four novel and biodegradable nano-systems of potential interest for MRI applications. In particular, MnO_2-Fe_3O_4 core-shell and MnO_2-Fe_3O_4 composites as a combination of MnO_2-Nano-sheets (NSs) or MnO_2-NPs and Fe_3O_4 NPs were synthetised. Raman spectra, Dynamic Light Scattering, Zeta potential, Magnetization curve, SEM, XPS, and UV-Vis were performed to characterize nanosystems properties. The biodegradability and immune-response were investigated in an in-vitro study to ascertain the bio-applications. Different exposure times of cells line to nanosystems were considered and new materials characterization were performed. The relaxivity measurements (T_1 and T_2) were carried on at high resolution MRI (3T). A 3D-phantom reporting nanosystems and precursors at different concentration in water solution were used. The Gd signals were used as reference in the relaxivity study. The role of shape, size and design were investigated and compared to define the best nanosystems performance.

Oral T4-4

Structural, magnetic and micromagnetic properties of $Dy_{1-x}Gd_xCo_3$ as a candidate for hosting ferrimagnetic skyrmions

R G Hategan[1], R Hirian[1], Z T Ludmaj[1], A Aldea [1], R D Miclea [1] and C Tiusan[1,2]

[1] Babes-Bolyai University, Faculty of Physics, Department of Condensed Matter Physics and Advanced Technologies, 1 M. Kogalniceanu, 400084, Cluj-Napoca, Romania

[2] National Center of Scientific Research, 54000 Nancy, France

E-mail: radu.hategan@ubbcluj.ro

Abstract. One of the most recent challenges in both classic and quantum information technologies is based on device implementation of topological magnetic textures such as magnetic skyrmions. Within this context, our studies cover the area of ferrimagnetic materials based on Rare-Earth – Transition-Metal (RE-TM) alloys in structural configurations providing tuneable ferrimagnetism: net magnetization, compensation temperatures. Here we focus on the ferrimagnetic intermetallic $Dy_{1-x}Gd_xCo_3$ system for which the bulk structural and magnetic properties were investigated for x ranging from 0 to 1. The samples were prepared by arc-melting under an argon atmosphere and annealed. X-ray diffraction analysis revealed and confirmed the expected structural properties of the system. The main magnetic properties (saturation magnetization and magnetic anisotropy) and their temperature dependence were determined through vibrating sample magnetometry. By performing DFT calculations and comparing them to the experimental results, we confirm the ferrimagnetic order of our compounds. Furthermore, using the experimental magnetic parameters, we performed micromagnetic simulations based on the dynamic Landau-Lifshitz-Gilbert (LLG) equation. These simulations reveal the parameter range (magnetic field, temperature, saturation magnetization, anisotropy, anti-symmetric exchange) in which the skyrmions can be stabilized in our materials. These issues are particularly important for classic and quantum applications of ferrimagnetic skyrmions.

Oral T4-5

From Imaging to Therapy: Curcumin-functionalized magnetic nanoparticles for dual MRI/Fluorescence imaging and photodynamic therapy

R Lapusan[1], A Balmus[1,2], S Dragan[3], R Fechete[4,5], R Borlan[2], M Focsan[1,2]

[1] Biomolecular Physics Department, Faculty of Physics, Babes-Bolyai University, 1 M. Kogalniceanu Street, 400084, Cluj-Napoca, Romania
[2] Nanobiophotonics and Laser Microspectroscopy Centre, Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, 42 T. Laurian Street, 400271, Cluj-Napoca, Romania
[3] Doctoral School of Integrative Biology, Department of Molecular Biology and Biotechnology, Faculty of Biology and Geology, Babeș-Bolyai University, 4-7 Clinicilor Street, 400006 Cluj-Napoca, Romania
[4] INSPIRE Platform, Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, 11 A. Janos Street., 400028, Cluj-Napoca, Romania
[5] Physics and Chemistry Department, Faculty of Material and Environmental Engineering, Technical University of Cluj-Napoca, 103-105 Muncii Avenue, 400641, Cluj-Napoca, Romania

E-mail: raducristianlapusan@gmail.com

Abstract. Magnetic nanoparticles are widely explored as MRI contrast agents, yet their clinical translation requires improved biocompatibility and multifunctionality. In this study, we first assessed ultrasmall magnetic nanoparticles (9.2 ± 2.9 nm) in agarose-based phantoms, demonstrating excellent contrast performance compared to the clinical agent Gadovist on a 1.5 T MRI system. To enhance in vivo applicability, the nanoparticles were coated with bovine serum albumin (BSA), resulting in size-tunable constructs with significantly improved performance in relaxometry studies. BSA not only enhances biocompatibility but also offers versatile surface chemistry, enabling further functionalization. We conjugated the BSA-coated nanoparticles with curcumin to create dual-modality nanoagents. Curcumin provides intrinsic fluorescence for real-time intraoperative guidance and acts as a reactive oxygen species (ROS) generator upon light activation, enabling photodynamic therapy (PDT). In vitro evaluation using a colorectal cancer cell line confirmed high cellular uptake and excellent biocompatibility, supporting the potential of these nanoparticles as safe, multifunctional theranostic tools. This work advances the design of magnetic nanoparticles beyond MRI, integrating optical imaging and PDT capabilities to support pre-operative diagnosis and intraoperative treatment within a single nanoplatform.

Oral T4-6

Modelling 2D Nanoflake - Bacterium Interactions in Solutions

N Leto[1], J Adam[1], A M Chiariello[1], M Singh[2], M Valadan[3], M R Del Sorbo[1], S Bianco[1], C Altucci[1], M Nicodemi[1]

[1] University of Naples Federico II, Naples, Italy

[2] Politecnico di Milano, Physics Department, Milan, Italy

[3] Consiglio Nazionale delle Ricerche, Istituto di Chimica Biomolecolare, Via Campi Flegrei 34, 80078 Pozzuoli NA, Italy

E-mail: nicolasleto.11@gmail.com

Abstract. Understanding the interaction between nanomaterials and biological membranes is crucial for advancing applications in nanomedicine and antimicrobial therapies. Nanomaterials such as MoS_2 and WS_2 nanoflakes exhibit unique physical properties that could be used for biomedical applications.

This study aims to investigate the interaction dynamics between a bacterium such as Staphylococcus aureus (S. aureus), potentially responsible for some important pathologies such serious forms of pneumonia, and two-dimensional (2D) nanoflakes of MoS_2 and WS_2. The model, based on Molecular Dynamics (MD) simulations, takes into account the material type, its affinity with the bacterial culture, and the concentration of the nanoflakes relative to the bacteria in solution. We performed MD simulations using LAMMPS. The bacterium was modelled as a static spherical entity, while the nanoflakes were treated as 2D squares composed of 9 nanoparticles. Harmonic potentials line lowed 3D motion in fluid. Simulations were conducted for MoS_2 and WS_2 nanoflakes, with interaction potentials of -7.4 kT and -5 kT, respectively. The study shows that nanoflake material and concentration significantly influence the interactions with and the dynamical approach to the bacterial surface, with MoS_2 and WS_2 displaying distinct behaviours. These insights help potential advance in the use of nanomaterials as antimicrobial agents.

Oral T4-7

Engineering hybrid nanostructures via self-assembly of janus nanoparticles and polymersomes for biomedical applications

V Mihali[1,2] and C G Palivan[1,2]

[1] Department of Chemistry, University of Basel; Mattenstrasse 22, 4002 Basel, Switzerland

[2] NCCR Molecular Systems Engineering; Mattenstrasse 22, 4002 Basel, Switzerland

E-mail: voichita.mihali@unibas.ch

Abstract. A significant approach in various fields such as chemistry, electronics, and technology are the self-organization of nano-objects into complex architectures. This strategy aims to generate novel systems with unique properties and functionalities. An important step in creating interconnected artificial organelles is the DNA hybridization between synthetic assemblies, including polymersomes, nanoparticles, and micelles. These assemblies facilitate cascade reactions among different encapsulated catalytic compounds and can imitate cell signaling and interactions. In this study, a new approach is proposed for developing a multifunctional hybrid system for specific bio-applications by investigating the self-organization of clusters between "hard" Janus nanoparticles (JNPs) and "soft" polymersomes. These polymer-based JNPs provide an asymmetric platform suited for directional interaction with soft polymersomes. The asymmetry of the JNPs has unique advantages by allowing a precise arrangement of the polymersomes and enabling, in a modular manner, various reaction configurations, including single, parallel and cascade enzymatic reactions. Additionally, these clusters, which integrate imaging and therapeutic nanocompartments, support nanotheranostic applications by enabling precise in vitro detection and simultaneously producing reactive oxygen species (ROS) to induce apoptosis.

Oral T4-8

Eco-friendly biochar-metal oxide adsorbents for emerging contaminant removal

C Mormile[1], O Opriş[2], I Lung[2], A Stegarescu[2], I Kacso[2], A Turza[2], S Tripon[2], S Pintea[2], S Bellucci[1], R Sturza[3], A Ghendov-Moșanu[3] and M L Soran[2]

[1] R.A.I.T. 88 S.R.L, Via Pieve Torina, 64/66, 00156 Rome, Italy

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

[3] Faculty of Food Technology, Technical University of Moldova, 9/9 Studenților St., MD-2045 Chișinău, Moldova

E-mail: mormile@rait88.com

Abstract. In response to growing environmental concerns, this study explores the development of sustainable adsorbent materials for water purification. A novel method is presented for converting apple waste into activated biochar (A-ac), which is further enhanced with green-synthesized metal oxides (Fe_3O_4 and NiO). Three hybrid materials A-ac-Fe_3O_4-ext, A-ac-NiO-ext, and A-ac-Fe_3O_4-NiO-ext—were synthesized and thoroughly characterized for their structural, morphological, and surface properties. These materials exhibited high specific surface areas ranging from 426.9 to 681.6 m^2/g. Preliminary adsorption experiments were conducted to evaluate their efficiency in removing emerging pollutants such as paracetamol, tartrazine, and industrial phthalates (DBP and DEHP) from synthetic water. Among the tested materials, A-ac-Fe_3O_4-ext demonstrated the best performance, achieving removal rates of up to 74.98% for DBP, 57.54% for paracetamol, and 37.48% for tartrazine. These findings highlight the synergistic interaction between biochar and metal oxides, which enhances adsorption capabilities. The study underscores the potential of these biochar-based composites as low-cost, eco-friendly materials for environmental remediation, while offering a sustainable approach to valorize agricultural waste and support the development of green technologies for advanced water treatment.

Oral T4-9

A UV-driven mof strategy to remove harmful pesticide residues from agricultural water

V C Niculescu, S L Badea, E I Geana and C Sandru

National Research and Development Institute for Cryogenic and Isotopic Technologies-ICSI Rm. Valcea, 4th Uzinei Street, 240050 Rm. Valcea, Romania

E-mail: violeta.niculescu@icsi.ro

Abstract. The removal of phenolic components originating from pesticide residues from water is of growing environmental concern due to their toxicity and persistence. This study focused on the targeted degradation of phenol, a key structural unit in many pesticides, using a photocatalytic system based on an iron-based metal-organic framework (Fe-BTC) activated under UV light. Fe-BTC was synthesized via a modified hydrothermal method and extensively characterized, revealing a micro-mesoporous structure with high specific surface area (360 m^2/g) and uniform particle morphology. The photocatalysis was performed under UV irradiation (365 nm) in the presence of H_2O_2, using 10 mg and 20 mg Fe-BTC as catalyst doses. The phenol and degradation products were monitored using HPLC-DAD. Rapid degradation was observed, with phenol dropping below the detection limit after 60 min in the first experiment and 45 minutes in the second. Major intermediates included hydroquinone, p-benzoquinone, and catechol, commonly associated with hydroxyl radical-induced oxidative pathways. A new degradation product (2.120 min) was tentatively attributed to pyrogallol, suggesting the potential formation of muconic acid intermediates. The findings demonstrated the effective removal of phenolic pesticide components through photocatalytic oxidation using Fe-BTC, emphasizing the synergistic role of UV light and H_2O_2 in activating the process. These results support the potential application of Fe-BTC in water treatment strategies targeting hazardous phenolic pollutants. Further studies are required to elucidate the complete degradation pathway and optimize catalyst performance.

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Oral T4-10

Bowl-inversion of corannulene-hybrid nanographenes

R A Saikia[1] **and M C Stuparu**[1,2]

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

[2] School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, 21 Nanyang Link 637371, Singapore

E-mail: raktim.saikia@itim-cj.ro

Abstract. Curved polyaromatic hydrocarbons, such as corannulene and sumanene, exhibit unique bowl-shaped molecular geometries that give rise to bowl-inversion dynamics. Identifying the bowl-inversion energy is essential for gaining prior insight into the chiral resolution of their derivatives and then, designing of chiral bowl aromatics. Thanks to variable-temperature (VT) ^{1}H NMR spectroscopy, which serves as a powerful technique to study the dynamic behavior of such aromatics. Corannulene exhibits a bowl-inversion barrier of 10.5–11.0 kcal/mol and undergoes rapid convex–concave inversion at room temperature. In this study, we examined the bowl-inversion dynamics of several corannulene-annulated nanographenes and demonstrated how pendant aryl groups can serve as effective NMR probes for investigating these dynamic processes. π-Extension at the periphery of the corannulene core contributes to increased rigidity and partial stabilization of its curved geometry. As a result, the *ortho*- and *meta*-protons of the pendant aryl groups become diastereotopic due to the asymmetry introduced by the curved environment. This diastereotopic nature was leveraged to monitor bowl-inversion behavior using 1D VT-^{1}H NMR. The experimental observations were further supported by density functional theory (DFT) calculations, which provided complementary insights into the inversion mechanisms. Notably, four of the studied compounds exhibited bowl-inversion barriers exceeding 18 kcal/mol, a remarkable finding.

Oral T4-11

In vitro efficacy of curcumin-loaded polymer films based on hyaluronic acid against melanoma cancer cells

P Snetkov[1], K Zavkibekova[2], A Motorzhina[2], R Shaikenov[1], P Serbun[1], K Levada[2], S Morozkina[1]

[1] Institute of Advanced Data Transfer Systems, ITMO University, Kronverkskiy Prospekt, 49, bldg. A, 197101 Saint Petersburg, Russia

[2] Institute of High Technology, Immanuel Kant Baltic Federal University, ul. A. Nevskogo, 14, 236016 Kaliningrad, Russia

E-mail: ppsnetkov@itmo.ru

Abstract. Melanoma is one of the oncological diseases with poor prognosis because of non-detection at the early stages, tendency to the metastases formation, and limited therapy. Natural biologically active compounds have a great therapeutic potential against cancer cells, with low levels of side effects. However, its hydrophobic nature leads to the poor water solubility and low bioavailability, which hinders its application. To overcome these drawbacks, various polymers and biopolymers can be used for the encapsulation of small molecules. In this study, the curcumin-loaded films based on hyaluronic acid with various molecular weights (1300 kDa, and 2480 kDa) were evaluated against lightly pigmented human melanoma SK-MEL 28 in comparison with the immortalized human keratinocytes HaCaT. Polymer films demonstrated a high level of inhibitory activity against SK-MEL 28 and high biocompatibility with the HaCaT cell line. These results obtained demonstrate the high potential of the application of thin and elastic curcumin-loaded polymer films as novel anticancer drug delivery systems with local (transdermal) administration. Moreover, it is supposed that combination of several pharmaceutical agents into the polymer matrix based on hyaluronic acid can lead to a synergetic effect of action. This research was funded by the Russian Science Foundation, project number 24-23-00269.

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Oral T4-12

Nonstabilizerness in many-body quantum systems

D Sticlet

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

E-mail: doru.sticlet@itim-cj.ro

Abstract. Understanding the origin of quantum advantage remains a central challenge in contemporary quantum science. A promising direction in this endeavor involves quantifying non-classical resources through the so-called nonstabilizerness Rényi entropy, commonly referred to as *magic* [Phys. Rev. Lett. 128, 050402 (2022)], which captures the deviation of a quantum state from the set of stabilizer states. We explore the generation and dynamics of *magic* in quantum many-body systems, focusing on one-dimensional spin chains where matrix product states techniques enable efficient simulations. Specifically, we examine the *magic* in one- and two-particle quantum walks where the evolution is governed by the XXZ Hamiltonian. Here we uncover light-cone dynamics of excitations accompanied by logarithmic growth of *magic*. In the long-time limit, after the light-cone reaches the system edges, magic stabilizes to a constant value with significant finite-size fluctuations. We also study open quantum system dynamics in boundary-driven and dephasing XXZ models described by Lindblad equations. Our analysis reveals new behaviors of magic, including sharp signatures of different transport regimes, universal scaling, and transient enhancements. Furthermore, we quantify how many-body correlations contribute to the growth of magic during system's evolution. These findings highlight magic as a sensitive and informative probe of non-equilibrium quantum dynamics.

Oral T4-13

Tunable hybrid microcapsules loaded with gold nanoparticles for photothermal therapy

D Stoia[1,2], A Holca[1,2], S Grecu[3] and M Focsan[1,2]

[1] Biomolecular Physics Department, Faculty of Physics, Babes-Bolyai University,1 M. Kogalniceanu Street, 400084, Cluj-Napoca, Romania

[2] Nanobiophotonics and Laser Microspectroscopy Center, Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, 42 Treboniu Laurian Street, 400271, Cluj-Napoca, Romania

[3] Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, 42 Treboniu Laurian Street, 400271, Cluj-Napoca, Romania

E-mail: daria.stoia@ubbcluj.ro

Abstract. Developing effective photothermal agents is key to advancing minimally invasive, selective cancer therapies. This study presents a hybrid microsystem for enhanced photothermal therapy by integrating gold nanoparticles (GNPs) into polymeric microcapsules (MCs), forming plasmonic-polymeric microcapsules (PPMCs). Two gold nanostructures—spherical (AuNPs) and rod-shaped (AuNRs)—were synthesized and loaded into MCs *via* the layer-by-layer deposition technique, achieving high loading efficiencies (86.7% for AuNPs, 94.4% for AuNRs). Dark-field and scanning electron microscopy confirmed the spherical morphology and successful internalization of GNPs. These nanoparticles, optimized for visible and near-infrared absorption, enhance light-to-heat conversion for surface and deep tissue therapy. The biocompatible MCs offer stability and potential for controlled drug release. PPMCs demonstrated photothermal responsiveness under laser exposure (532, 680, 730, and 808 nm) with real-time temperature imaging. To extend functionality, the near-infrared fluorophore Indocyanine Green (ICG) was incorporated into the polyelectrolyte layers, enabling fluorescence imaging. Conventional fluorescence microscopy confirmed successful ICG loading. This multifunctional PPMC system holds promise for precise, tunable photothermal therapy and imaging.

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Oral T4-14

Assessment of the role of strong metal-support interaction on electrocatalytic performance of composite supported Pt catalysts

Z Pászti, I Borbáth, C Silva and A Tompos

Institute of Materials and Environmental Chemistry, HUN-REN Research Centre for Natural Sciences, Magyar Tudósok körútja 2, H-1117 Budapest, Hungary

E-mail: tompos.andras@ttk.hun-ren.hu

Abstract. Interactions between metals and supports are gaining more attention because of their ability to tune the physicochemical properties of catalysis. Strong metal-support interaction (SMSI) significantly impacts catalyst performance through geometric, electronic and bifunctional effects, influencing catalytic activity, selectivity and stability. SMSI usually results in electron transfer between the metal and the oxide, accompanied by the decoration of the metal particles with ultra-thin layers of the support material upon hydrogen pre-treatment. This work focuses on the development of SMSI and its impact on the catalytic performance of the Pt/$Ti_{0.8}Mo_{0.2}O_2$-C system design for use in polymer electrolyte membrane fuel cells. Beneficial metal-support interactions developing at the Pt-oxide-carbon junctions contribute to higher activity and better stability of the catalysts, which may allow design of effective electrodes with decreased Pt content. By comparing the structural and electrochemical features of electrocatalysts reduced at different temperatures, it was found that pre-treatment at 250 °C-350 °C is the optimal for enhancing the performance of this catalyst family.

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Poster T4-1

Sustainable valorization of spent coffee grounds: production and activation of high-performance biochar

A Balla, C Marcu, C Lar, M Miheţ, S Tripon, I Kacsó, X Filip, A Turza, C Leoştean and J Z Szücs-Balázs

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

E-mail: ancuta.balla@itim-cj.ro

Abstract. Spent coffee grounds (SCG) represent a readily available waste resource with great potential for valorisation into functional materials. In this study, we report the production of biochar from SCG through pyrolysis at 850 °C under an inert atmosphere. The resulting biochar was further activated using different post-treatment strategies, including chemical activation (acid/base treatments) and physical activation (steam and CO_2). We systematically investigated how these activation methods influence the surface area, porosity, and surface functional groups of the SCG-derived biochar, employing techniques such as BET, SEM, NMR, FTIR and XPS analysis. The activated biochar was evaluated for their potential in environmental applications, such as adsorption of pollutants or catalytic support materials. Our results demonstrate that the combination of high-temperature pyrolysis and tailored activation produces yields biochar with optimized surface characteristics and designed functionalities, offering a sustainable pathway for the circular utilization of coffee waste.

Poster T4-2

Development of a portable sers-based biosensor for sensitive detection of cyanotoxins in freshwater sources

I A Brezeştean, D Marconi, A Colniță, A S Tătar and N E Dina

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

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

Abstract. Biosensors, particularly those utilizing Surface-Enhanced Raman Scattering (SERS) spectroscopy, have become powerful tools for detecting compounds and (bio)molecules at trace-level. Meanwhile, water quality is significantly deteriorating due to agricultural and industrial runoff, and untreated sewage into our freshwater sources. Continuous monitoring of these aquatic systems is essential to maintain water quality, highlighting the crucial role of sensor technologies in pollutant detection.

In this study, we present technical parameters such as device dimensions, structural configuration, sample volume, and architecture of the demonstrator, using CAD-based 2D and 3D technical drawings of the components' architecture developed to support the fabrication and assembly process.

The experimental demonstrator incorporates an innovative SERS-based detection concept aimed to detect cyanotoxins in regional stagnant waters, particularly in the context of uncontrolled algal blooms. Herein, we fabricated SERS-active substrates using advanced nanofabrication techniques such as Nanoimprint Lithography (NIL) and Magnetron Sputtering (MS), and then evaluated the performance of the in-house fabricated system by employing a portable Raman spectrometer to detect standard analytes such as Crystal Violet, Adenine, and Rhodamine. This work represents a promising step toward the deployment of reproducible, flexible, field-ready biosensors for real-time environmental monitoring.

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Poster T4-3

Structural and transport analysis of materials for superconducting qubits in Josephson junctions

L Buimaga-Iarinca, T Murariu, C Tripon and C Morari

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

E-mail: luiza.iarinca@itim-cj.ro

Abstract. Understanding the individual impact of structural factors such as defects, disorder, pressure, and temperature on materials at the nanoscale is often challenging in experimental settings. Computational modeling offers a powerful alternative to disentangle these contributions and guide material design. Our group specializes in the numerical evaluation of material properties, employing methods ranging from density functional theory (DFT) to molecular dynamics (MD). Recent work has focused on three key areas: (i) supporting experimental development of next-generation battery materials, (ii) investigating materials for quantum technologies—particularly superconducting qubits, and (iii) analyzing molecule–metal surface interactions. In this contribution, we present results from DFT and MD simulations of aluminum oxide nanostructures, highlighting their relevance in the fabrication of Al–AlOx–Al Josephson junctions for superconducting quantum circuits. These computational results support experimental efforts within the QuCos QuantERA project.

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Poster T4-4

Heavy metal adsorption by waste-derived magnetic sorbents

A Bunge, I-V Ganea and C Leostean

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

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

Abstract. More and more in the last years, polluted water and the necessity to purify natural water sources to obtain drinking water have become a major problem in today's society. Magnetic sorbents have recently found wide popularity in the research concerning water purification. In most cases, however, at least the magnetic part of the sorbent is synthesized using non waste derived starting materials. Here, a series of magnetic sorbents synthesized using only waste materials was used to adsorb heavy metals from waste water. The materials were characterized using SEM-EDX, FTIR and VSM measurements, and the adsorption process researched in detail. Additionally, differences in the sorption capacity of a series of different heavy metals are shown.

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Poster T4-5

Antibiotics removal using materials based on biochar

A M Chiş[1], O Opriş[1], I Lung[1], A Stegarescu[1], I Kacso[1], A Turza[1], S Tripon[1], S Pintea[1], C Mormile[2], S Bellucci[2], R Sturza[3], A Ghendov-Moșanu[3], H Y Dasgan[4] and M L Soran[1]

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

[2] R.A.I.T. 88 S.R.L, Via Pieve Torina, 64/66, 00156 Rome, Italy

[3] Faculty of Food Technology, Technical University of Moldova, 9/9 Studenților St., MD-2045 Chișinău, Moldova

[4] Department of Horticulture, Agricultural Faculty, Cukurova University, 01330 Adana, Türkiye

E-mail: anda.chis@itim-cj.ro

Abstract. Antibiotics are pharmaceutical compounds, wide used in medical treatments. These compounds may be found in waters, such as rivers and in wastewater. Therefore, it is necessary to find an efficient solution for removing them from water. From the methods used for antibiotics removal, one efficient method is adsorption. As adsorbent can be used a material based on biochar and biopolimers, that combines the properties of them. Biochar is a carbon based material obtained from vegetable residues, that has good adsorbent properties for these compounds. In this study, the biochar from apple wastes was prepared and the encapsulated biochar in polymer was tested for ciprofloxacin and norfloxacin removal from aqueous solutions. For both antibiotics the adsorption parameters like contact time (5-40 min), antibiotic concentration (5-80 mg/L) and temperature (20-40°C) were optimized. The best removal degree for ciprofloxacin (100%) was obtained at 40 min, 40 mg/L and 25°C, and for norfloxacin at 15 min, 5 mg/L and 25°C.

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Poster T4-6

Green synthesis of fluorescent Carbon Dots by microwave-assisted facile route

D Cisternino[1], F Delle Fave[1], M Froio[1], A Leone[2], N Ucciardello[1] and P G Medaglia[1]

[1] Department of Industrial Engineering, University of Rome “Tor Vergata”, Rome, I-00133, Italy

[2] Department of Electronic Engineering, University of Rome “Tor Vergata”, Rome, I-00133, Italy

E-mail: cisternino.diego@gmail.com

Abstract. In this work we present the preliminary results concerning the synthesis of fluorescent carbon dots. These nanostructured systems, mainly Graphene Quantum Dots (GQDs) have been obtained starting from green precursors like urea and citric acid by optimizing a facile, cheap and efficient microwave-assisted hydrothermal route. The morphological, structural and physico-chemical features of obtained nanostructures, characterized by different techniques, confirm that they could open promising perspectives for possible applications.

Poster T4-7

Controlling Surface-Enhanced Fluorescence via Spacer Layer Engineering on Nanostructured Films

A Falamas[1], I Cardan[1], D Cuibus[1], N Tosa[1], A Rostas[1], S Boca[1,2], and C Farcau[1]

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

[2] Interdisciplinary Research Institute in Bio-Nano-Sciences, Babes-Bolyai University, 42 Treboniu Laurian, 400271 Cluj-Napoca, Romania

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

Abstract. This study investigates the role of spacer layers in controlling surface-enhanced fluorescence (SEF) from quantum dots (QDs) and small fluorophores on nanostructured thin films. To minimize quenching and modify the emitter–nanostructured film distance, various interlayers were evaluated, including polymer matrices (PVA, PVP), and polyelectrolytes. Gold films over nanospheres (AuFoN) served as metallic SEF substrates for CdSe/ZnS QDs embedded in PVA, with fluorescence enhancement depending on nanosphere size. In parallel, ZnO nanostructures-based thin films fabricated by drop-coating were used as semiconductor platforms for spin-coated Nile Blue in PVP, where enhancement correlated with film morphology and polymer concentration. Further, the potential of these developed platforms for SEF-based biosensing applications, either in liquid or as solid substrates, is explored. These findings highlight the critical role of interfacial engineering—whether through polymeric spacers or emitter–analyte design—in modulating SEF and enabling future sensing strategies.

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Poster T4-8

Green Chemistry in Action: Removing Dyes Using Waste-Based Materials

I-V Ganea[1,2], A Nan[1], M Dan[1] and A. Bunge[1]

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

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

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

Abstract. Synthetic dyes are widely used in different industries such as textiles, printing, and cosmetics, often ending up in wastewater where they pose serious environmental and health risks due to their toxicity and persistence. Effective removal of these pollutants is crucial for protecting aquatic ecosystems and human health. In this context, the present study explores the potential of two novel composite materials synthesized from food and industrial waste for removing crystal violet (CV) dye from aqueous solutions. The new composites were first characterized by FTIR, TGA and SEM and further applied in the adsorption of CV. Preliminary adsorption tests assessed the impact of initial dye concentration and contact time on removal efficiency and sorption capacity of the composites. At low concentrations (≤10 mg/L) the new materials achieved 100% removal within just 5 minutes. At higher concentrations (100–500 mg/L), the food-waste composite demonstrated significantly higher performance, reaching up to 96.9% removal, compared to a maximum of 80.1% for the composite including industrial waste. Kinetic analysis indicated that pseudo-second-order model best fit the data, suggesting chemisorption as the dominant mechanism. These results highlight the potential of sustainable, low-cost materials derived from food and industrial waste for rapid and efficient wastewater treatment applications.

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Poster T4-9

Towards Designing Antibacterial Materials Based on Cysteine

O Grad, A Khan

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

E-mails: oana.grad@itim-cj.ro; anzarul.khan@itim-cj.ro

Abstract. Cysteine is the only natural amino acid that contains a thiol functionality. The thiol group can participate in disulfide formation and complexation with metal atoms. Hence, cysteine plays a key role in the structure stabilization of proteins and facilitates enzymatic reactions involving a metal cofactor. Cysteine, thus, is an appealing building block for material synthesis. We hypothesized that the sulphur atom could be transformed into a sulfonium cation through consecutive alkylation reactions. This would lead to the preparation of cysteine-based electrolytes containing alkyl chains with membrane penetration properties, the zwitterion to enhance compatibility with mammalian cells, and the sulphur cation for disruption of bacterial cell membranes through electrostatic interactions. Thus, we began by developing an efficient synthetic route to the hypothesized materials. The first step could be achieved using thiol-epoxy 'click' chemistry with a variety of epoxide substrates. The reaction occurred in water and resulted in quantitative conversions of the starting materials into the targeted thioethers. Efforts are currently underway to transform the thioethers into sulfonium salts. Once accessed, their biological properties will be examined. In this poster presentation, our focus will be on discussing the synthetic feasibility of such cysteine-based cationic antibacterial materials.

Poster T4-10

Biocompatibility and Anticancer Effects of Manganese-Doped Copper Oxide Nanoplatelets in Cell Culture Models

S Guțoiu[1], I O Pană[1], S Boca[1,2,*], I Kacso[1], M O Miclăuș[1], O Grad[1], A M R Gherman[1], C Leostean[1], A Ciorîță[1,3,#] and M Suciu[1]

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

[2]Interdisciplinary Research Institute in Bio-Nano-Sciences, Babes-Bolyai University, 42 Treboniu Laurian, 400271 Cluj-Napoca, Romania

[3]Electron Microscopy Center C. Craciun, Faculty of Biology and Geology, Babes-Bolyai University,5-7 Clinicilor Street, 400006 Cluj-Napoca, Romania

[*] For these authors the primary affiliation is 2.

[#] For these authors the primary affiliation is 3.

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

Abstract. Cell–nanomaterial interactions are crucial for advancing diagnostic and therapeutic technologies. Comprehensive characterization of any engineered product requires evaluating its effects on specific biological systems, including observing cellular responses to material exposure. This study examined the biological effects of manganese-doped copper oxide (CuO:Mn) nanoplatelets on human BJ fibroblasts and A375 melanoma cells. The nanoparticles, synthesized at room temperature via a hydrothermal method, were thoroughly characterized using XRD, electron microscopy, XPS, and DLS. The analyses revealed flat, nanoscale structures with sharp edges, confirmed the formation of crystalline CuO, and provided insights into successful manganese incorporation. The findings indicate that nano-platelets interact with cells actively by mediating essential molecular processes.

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Poster T4-11

Conductive composite films based on polypyrrole suitable for various applications

G Ispas, A Andrei, M Zagrai, L Barbu-Tudoran, R P Turcu, and I Craciunescu

National Institute for Research and Development of Isotopic and Molecular

E-mail: george.ispas@itim-cj.ro

Abstract. This study discusses the synthesis of conductive composite films based on doped polypyrrole (PPy) and functionalized with polyethylene glycol (PEG) and/or graphene. A simple polypyrrole film is used as a reference material to evaluate the structural and functional changes resulting from the added components. Three types of composite films were developed and analyzed: polypyrrole-PEG, polypyrrole-graphene, and polypyrrole-PEG-graphene. This comparison highlights the impact of each component on the final properties of the materials. The conductive composite films were synthesized via electrochemical polymerization in the presence of specific fillers (PEG, graphene) and subsequently processed into freestanding films with excellent mechanical and chemical resistance. Physicochemical characterization revealed good compatibility between the incorporated components. The mechanical, electrical, and structural properties were systematically evaluated to assess the impact of the selected dopants on the overall performance of the composite films. Based on the obtained results, these composite materials could be directed toward specific applications in fields such as flexible electronics and sensors, supercapacitors and energy storage, as well as tissue engineering and other biomedical applications.

Poster T4-12

New strategy to modify CuO-ZnO-Al_2O_3 catalysts for the improved direct hydrogenation of CO_2 to methanol

A M Kasza[1,2], M D Lazar[1], M Mihet[1]

[1] National Institute for Research & Development of Isotopic and Molecular Technologies - INCDTIM, 67–103 Donat Str., 400293 Cluj–Napoca, Romania
[2] Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, 11 Arany János Str., 400028, Cluj–Napoca, Romania

E-mail: angela.kasza@itim-cj.ro

Abstract. Hydrogenation of CO_2 to methanol (CO_2-to-MeOH) offers a promising approach for reducing CO_2 emissions and chemically storing energy within the "power-to-liquid" (P2L) concept, while also providing an alternative to conventional methanol production from synthesis gas. Despite its potential, CO_2-to-MeOH faces challenges such as thermodynamic limitations, the stability of CO_2, side reactions, and catalyst deactivation. Research has primarily focused on the development of catalysts, especially the widely studied Cu/ZnO/Al_2O_3 (CZA) system. Among the various strategies aimed at improving catalytic performance, the use of carbon-based materials appears to be a particularly versatile approach.

In this study, two types of carbon structures (C_{MOF}) derived from metal-organic frameworks (MOF), specifically MIL-53(Al), were used to modify the CZA catalysts. These carbon species differ in their alumina content and consequently possess different structural properties. The incorporation of such carbon materials can simultaneously increase the specific surface area, enhance copper dispersion, and — due to the hydrophobic nature of the carbon species— improve the catalyst's water resistance. We investigated and compared the effects of these two types of carbon on the physicochemical properties of the modified CZA catalysts, which may directly influence their catalytic performance in CO_2 hydrogenation to methanol.

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Poster T4-13

Carbon-based structures decorated with W doped SnO_2 nanoparticles for supercapacitor applications

C Leostean[1], A Rostas[1], M Stefan[1], D Toloman[1], A Popa[1], S Macavei[1], A U Ammar[1], D Lazar[1], A Varadi[1] and E Erdem[2]

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

[2] Faculty of Engineering and Natural Sciences, Sabanci University, Tuzla, Istanbul, 34956, Turkey

E-mail: cristian.leostean@itim-cj.ro

Abstract. In recent years, supercapacitor devices have gained significant potential in energy systems due to their enormous power density, competing favourably with conventional energy storage solutions. Various carbon-based structures such us graphene oxide (GO), reduced graphene oxide (r-GO), multi walled carbon nanotubes (MWCNT), activated carbon (AC) and g-C_3N_4 decorated with 0.5% W doped SnO_2 nanoparticles were used as electrode materials for high-performance supercapacitor devices. The nanocomposites were formed applying poly-allylamine hydrochloride (PAH) as a polymer linker at a weight ratio of carbon structures - SnO_2-0.5%W of 1:1. SnO_2-0.5%W nanoparticles were obtained by chemical precipitation. The effect of the carbon structures on the electrochemical properties was reported. The samples were characterized using X-ray diffraction, electron microscopy and Raman spectroscopy to obtain information on the structural and morphological environment. Electron paramagnetic resonance, X-Ray Photoelectron Spectroscopy and photoluminescence spectroscopy gave information on the defect environment of the materials. Finally, the electrochemical performance of the electrode materials was tested using cyclic voltammetry, electrochemical impedance spectroscopy, and galvanostatic cycling with potential limitations as testing techniques. The result obtained showed extremely positive trends for this type of electrode material.

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Poster T4-14

Enhancing the supercapacitive properties of SnO_2 nanoparticles by doping with V^{4+} ions

S Macavei[1], A Varadi[1,2], I Nesterovschi[1], A Ammar Uddin[1], D Toloman[1], M Stefan[1], L Barbu Tudoran[1], E Erdem[1], A Rostas[1] and A Popa[1]

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

[2] Doctoral School of Chemistry, Babes-Bolyai University, Cluj-Napoca, 400084, Romania

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

Abstract. Tin oxide SnO_2 is a crucial n-type semiconductor, characterized by high chemical stability and exceptional electrical properties, rendering it a promising candidate for electrode materials in energy storage applications, such as supercapacitors. Thus, a series of V-doped SnO_2 nanoparticles were synthesized and tested as electrode materials for supercapacitor applications. This study highlights the influence of dopant ions on the electrochemical properties of SnO_2 by varying the dopant V-ion concentrations. The successful incorporation of the V ions in the SnO_2 lattice was evidenced by X-ray diffraction and energy-dispersive spectroscopy and was confirmed by Raman spectroscopy. The SEM/TEM images reveal the polyhedral shape of the nanoparticles. The defect centers and V-ions oxidation state, introduced in the SnO_2 lattice, were evaluated by Raman, Electron Paramagnetic Resonance, and Photoluminescence spectroscopy. Symmetric supercapacitor devices were assembled using the obtained nanoparticles to evaluate the electrochemical response of undoped and V-doped SnO_2 materials. The sample with 0.5% V-ions exhibits the highest specific capacitance value of 162.43 F/g at a 2 mV/s scan rate. This suggests that adding V ions to SnO_2, even in small amounts, improves the material's electrochemical performance. The best performing sample shows excellent cyclic stability of about 99% retention after 2000 cycles.

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Poster T4-15

Instant coffee - unconventional exfoliation medium for the production of N/F co-doped graphenes applicable in the sulfamethazine detection

L Magerusan, F Pogacean, and S Pruneanu

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

E-mail: lidia.magerusan@itim-cj.ro

Abstract. Sulfamethazine (SMZ), a persistent antibiotic, can be frequently detected in different animal derived food products endangering the customers' health; therefore its detection and identification even at trace levels are of major importance. The current study reports the development of an easy and rapid electrochemical detection protocol for SMZ assay employing a graphene-based sensor. The sensor material consists in a nitrogen-fluoride co-doped graphene produced in an ecological and economical manner through direct exfoliation of high purity graphite rods, at low applied bias (6V) in instant coffee containing solution. The doping of the as-prepared material was obtained without the employment of any chemical precursors containing nitrogen or fluoride. The resulting material was thoroughly characterized from morphological and structural point of view before being employed in the development of a glassy carbon modified sensing surface. The efficiency of nitrogen-fluoride co-doped graphene material in sulfamethazine assay was tested using cyclic voltametric and amperometric approaches. The modified glassy carbon surface proved a remarkable enhancement of the electrocatalytic performances towards sulfamethazine compared to the bare surface. Under optimized experimental conditions, in pH 5 acetate buffer solution, the developed sensor showed a low detection limit 8.48 nM, over a wide linear range 28 nM – 41.04 µM. Furthermore, the practical usefulness of the constructed sensor was evaluated in real sample analysis using several commercially available milk samples, with promising outcomes.

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Poster T4-16

3D flexible metal/semiconductor nanostructured surfaces fabricated by nanoimprint lithography and pulsed laser deposition techniques

D Marconi[1], A Colniță[1], I Brezeştean[1] and L Barbu-Tudoran[2]

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

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

E-mail: daniel.marconi@itim-cj.ro

Abstract. Hybrid nanostructures composed of metals and semiconductors of various shapes, sizes and compositions, are highly sought-after functional materials. Today, various nanoscale objects are synthesized, manipulated, characterized and used in a multitude of scientific and technological applications. High-resolution nanotrenches are new, advanced and modern elements, frequently used due to their dependence on the optical property of shape and periodicity. Nanotrenches architectures have wide applications in photonics, electronics and biotechnology. 3D flexible nanotrenches arrays were fabricated by nanoimprint lithography (NIL) on a flexible and transparent substrate such as IPS, with 300, 400 500 and 600 nm pitch. For uniform nanotrenches imprinted in the substrate, the NIL process parameters were optimized. The ZnO thin films were deposited on the fabricated nanotrenches arrays with different pitches by pulsed laser deposition technique. The metallization with gold (Au) thicknesses of 15nm, 25 nm and 60 nm was made using magnetron sputtering deposition technique. The topography of ZnO and ZnO@Au thin films was assessed from Scanning Electron Microscopy (SEM) images.

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Poster T4-17

Utilization of modified spent coffee ground biochar for Cr(VI) adsorption from aqueous solutions

C Marcu, A Balla, C Lar and J-Z Szücs-Balázs

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

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

Abstract. The contamination of water sources by hexavalent chromium Cr(VI), a highly toxic and carcinogenic heavy metal, has a serious environmental threat. In this study, spent coffee grounds were utilized as a low-cost, sustainable precursor to produce biochar adsorbents, which were subsequently modified through various treatments to enhance their adsorption performance. The adsorption capacity of these modified biochar for Cr(VI) was systematically investigated under different initial concentrations (0.1 g/L – 0.3 g/L Cr) at room temperature. Batch adsorption experiments were conducted, and the Cr(VI) concentrations in solution were determined using UV-Visible spectrophotometric method. The results indicate that the modification of biochar significantly influences its surface properties and Cr(VI) removal efficiency. This work highlights the potential of valorizing agro-waste for the development of effective adsorbents for heavy metal remediation in water.

Poster T4-18

Manganese doped molybdenum sulfide nanoflowers for supercapacitor application

K Maškarić[1,2], D Toloman[1], A Rostas[1], A Popa[1], A U Ammar[1], M Stefan[1], S Macavei[1], A Varadi[1,3], E Erdem[1,4]

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

[2] Biomolecular Physics Department, Babes-Bolyai University, Kogalniceanu 1, Cluj-Napoca, 400347

[3]Doctoral School of Chemistry, Babes-Bolyai University, Cluj-Napoca, 400084, Romania

[4]Faculty of Engineering and Natural Sciences, Sabanci University, Tuzla, Istanbul, 34956, Turkey

E-mail: karlo.maskaric@itim-cj.ro

Abstract. Manganese (Mn) doped molybdenum disulfide (MoS_2) nanoflowers with various concentration of Mn were synthesized in this work using hydrothermal method. The synthesized material was used as an electrode material in supercapacitor application, elucidating the effects of Mn ions on the electrochemical properties. Characterization of the Mn doped MoS_2 nanoflowers with X-ray diffraction, electron microscopy, and Raman spectroscopy provided information about morphology and structure. Electron paramagnetic resonance, photoluminescence, Raman, and UV-Vis spectroscopy provided information about defects in the material, which is important as changes in the defect environment directly affect electrochemical properties. Electrochemical performance of the electrode material was tested in all-in-one supercapacitor devices using galvanostatic cycling with potential limitations, electrochemical impedance spectroscopy and cyclic voltametry. The 0.7% Mn-doped MoS_2 has shown the highest specific capacitance value of 1633.33 F/g at 2 mV/s scan rate, energy density of 226.9 Wh/kg, and cyclic stability of 68% after 2000 cycles.

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Poster T4-19

Friedel oscillations in a two-dimensional electron gas and monolayer graphene with a non-Coulomb impurity potential

L Máthé[1] and I Grosu[2]

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

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

E-mail: levente.mathe@itim-cj.ro

Abstract. We study Friedel oscillations in a two-dimensional non-interacting electron gas and in a monolayer graphene in the presence of a single impurity. The potential generated by the impurity is modelled using a non-Coulomb interaction ($\sim r^{-\eta}$). The charge carrier density deviation as a function of distance from the impurity is calculated within the linear response theory. Our results show that, in both a two-dimensional non-interacting electron gas and graphene, the phase of charge carrier density oscillations remains unaffected by the parameter η, which characterizes the non-Coulomb nature of the interaction, at large distances from the impurity. The parameter η influences only the amplitude of the oscillations in this regime. The results for an impurity modelled by Coulomb-like potential ($\eta = 1$) are recovered in both cases.

Poster T4-20

Ultrasensitive, label-free biosensing using large-area plasmonic nanostructures fabricated via nanosphere lithography

A C Maxim[1], I Mahboub[1,2], M L de la Chapelle[3] and M Focșan[1,2]

[1] Nanobiophotonics and Laser Microspectroscopy Centre, Interdisciplinary Research Institute on Bio-Nano-Sciences, Babeș-Bolyai University, Treboniu Laurian Street, 400271 Cluj-Napoca, Romania;

[2] Biomolecular Physics Department, Faculty of Physics, Babes-Bolyai University, Mihail Kogalniceanu Street, 400084 Cluj-Napoca, Romania;

[3] IMMM – UMR 6283 CNRS, Le Mans Université, Olivier Messiaen Avenue, 72085 Le Mans, France.

E-mail: andreea.carmen.maxim@ubbcluj.ro

Abstract. Most current diagnostic procedures are complex, invasive, and time-consuming, involving multi-step protocols. In this study, we develop an original plasmonic nanobiosensor for the ultrasensitive, label-free detection of disease-relevant proteins. Our innovative sensor ensures dual-mode detection, integrating two spectroscopic techniques—Localized Surface Plasmon Resonance (LSPR) and Surface-Enhanced Raman Scattering (SERS)—to enable precise molecular recognition. Using nanosphere lithography, we fabricated homogeneous hexagonal arrays of gold nanotriangles that act as plasmonic nanoplatforms, generating electromagnetic "hot spots" for Raman signal enhancement. These platforms enable detection based on the unique spectral fingerprints of biomolecules and demonstrate high sensitivity for complementary polynucleotides (PolyA / PolyT). We systematically validated the sensor's sensitivity, reproducibility, and signal uniformity through controlled testing with model sequences. This work represents a significant step forward in point-of-care diagnostics, providing a powerful tool for early disease detection and real-time clinical decision-making.

Poster T4-21

Green synthesis of silver nanoparticles using *Pistacia Lentiscus* leaf extract and evaluation of their antibacterial activity

K Mellouk[1], S Ouchenane[2] and L Ferchichi[1]

[1] Laboratory of Organic Synthesis and Biocatalysis, Chemistry Department, University Badji Mokhtar, Annaba, Algeria

[2] Laboratory of Inorganic Materials Chemistry, Chemistry Department, University Badji Mokhtar, Annaba, Algeria

E-mail: karima.mellouk@univ-annaba.dz

Abstract. This study reports the green synthesis of silver nanoparticles (AgNPs) using an extract from *Pistacia lentiscus* leaves as a natural reducing agent. The approach aims to develop pure, functional nanomaterials while avoiding toxic chemical reagents. The synthesized nanoparticles were characterized by X-ray diffraction, Fourier-transform infrared spectroscopy, scanning electron microscopy, and energy-dispersive X-ray spectroscopy. The analyses revealed spherical morphology, nanoscale crystallite size, and a crystalline structure consistent with reference data, confirming the successful synthesis. EDS results indicated high purity, with silver as the sole major element. The antibacterial activity of the AgNPs was evaluated against two resistant pathogenic bacterial strains, showing significant effectiveness, particularly against *Staphylococcus aureus*. These findings highlight the potential of green synthesis routes for producing nanostructured materials with functional properties, offering promising applications in biomedical and environmental fields.

Poster T4-22

Sustainable waste-based materials for mining water treatment

P S Mureșeanu[1], I-V Ganea[1,2], R Balc[1] and A Nan[2]

[1] Faculty of Environmental Science and Engineering, Babeș-Bolyai University, 30 Fantanele, 400294 Cluj-Napoca, Romania

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

E-mail: paulmureseanu70@gmail.com

Abstract. The mining sector in Romania during the socialist period has left behind a considerable environmental footprint, most notably in the form of polluted mining wastewater and tailings. Tailing ponds and abandoned mines continue to pose major environmental and human risks even today. In this context, there is a constant need for sustainable, "green" solutions that address the complex issue of mining wastewater decontamination. Considering the above, the current study aimed to prepare a new eco-friendly composite based on food and industrial wastes and further apply it in the removal of heavy metals from contaminated waters in Borșa mining perimeter (Maramureș County, Romania). The new material was characterized via FTIR, TGA and SEM-EDX and preliminary tested the effect of initial metal concentration, contact time, material dosage on the metal adsorption from stock solutions. The results showed that the adsorption efficiency reaches 98% for concentrations of Cu below 40 mg/L, when using 10 g of material after 4 hours of interaction with the contaminated solution. These findings demonstrate the potential application of the newly-developed waste-based composite in the mining water treatment sector.

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Poster T4-23

Next-generation modified PVDF membranes for enhanced efficiency in dye removal using photocatalysis and adsorption techniques

S Goia[2], A Bunge[1], A Popa[1], C Tudoran[1], A Nan[1]

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

[2]National College "Gheorghe Șincai", 33 Avram-Iancu, Cluj-Napoca, Romania

E-mail: alexandrina.nan@itim-cj.ro

Abstract. Contamination of wastewater by dye and pharmaceuticals poses a significant threat to both human health and the environment. During dyeing, industries such as paper, rubber, plastic, and textiles can lose between 1% and 50% of their dye concentration, releasing these substances into wastewater. In this study, we present the modification of PVDF membrane using poly(benzofuran-co-arylacetic acid) (PBAAA) and poly(benzofuran-co-arylacetic acid) functionalized with dopamine (PBAAA-DA) to improve the immobilization of ZnO nanoparticles on its surface. The modifications were achieved through straightforward adsorption of PBAAA and PBAAA-DA, as well as spin-coating techniques. We utilized cold plasma treatment to effectively clean and activate the surfaces of the PVDF membranes prior to the deposition of PBAAA. We developed several distinct types of membranes: PVDF-PBAAA-ZnO and PVDF-PBAAA-DA-ZnO. PBAAA was chosen for its ease of preparation and its high degree of functionalization, including various reactive groups such as phenol, carboxylic acid, and lactone. These properties make PBAAA a versatile polymer for linking different types of functionalities in an orthogonal manner. By functionalization, the membranes' hydrophilicity was enhanced. These membranes were tested for removing Rhodamine B dye from water by adsorption and photocatalytic processes under UV-light irradiation.

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Poster T4-24

Synthesis and characterization of graphene–metal oxide materials using plant extracts for the preliminary adsorptive removal of pesticides from aqueous solutions

O Opriş[1], A Stegarescu[1], I Lung[1], M Mihet[1], I Kacso[1], A. Turza[1], S Tripon[1], T Tata[2], P G Medaglia[3], C Leonardi[3], M L Soran[1]

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

[2] Environment and Biodiversity Research Division, Environmental Research Center, Alzon Castle, Boughazi Said Street, Annaba,23005, Algeria

[3] Department of Electronic Engineering, University of Rome "Tor Vergata", Rome, I-00133, Italy

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

Abstract. The presence of various organic and inorganic contaminants in water sources is concerning because of their toxicity, persistence, and often high concentrations. In response, extensive research is being directed toward developing effective treatment methods and technologies for environmental remediation. Among these, nanotechnology has emerged as a promising approach, due to nanomaterials that have large specific surface areas and excellent adsorption properties, making them highly effective for pollutant removal. The present study aimed to obtain materials based on graphene obtained from hemp and functionalized with metal oxides (CuO, Fe_3O_4) using plant extracts (apple and carrot wastes, and *Urtica dioica* L.), and their testing in water decontamination. The obtained materials were characterized using the Brunauer-Emmett-Teller method, X-ray diffraction, transmission/scanning electron microscopy, and Fourier transform infrared spectroscopy. Functionalizing graphene with metal oxides using plant extracts enhanced its adsorption efficiency for the removal of pesticides from aqueous solutions, achieving removal degrees up to 97% for cymoxanil and 95% for triadimefon. These preliminary results highlight the potential of green-synthesized graphene–metal oxides as an efficient and sustainable material for the adsorptive removal of water contaminants, contributing to the advancement of eco-friendly water treatment technologies.

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Poster T4-25

Interfacial electron transfer between half-metals and transition metal dichalcogenides

O Pana[1], M Stefan[1], D Toloman[1], S Macavei[1], C Leostean[1], S Gutoiu[1], C M Teodorescu[2], S Colis[3]

[1] Natl. Inst. for R&D. of Isotopic and Molec. Technol., 67-103 Donat, 400293 Cluj-Napoca, Ro.

[2] Natl. Inst. of Mater. Phys., Atomiștilor 405A, 07715 Măgurele–Ilfov, Ro.

[3] Univ. Strasbourg, Inst. Phys. & Chem. Mater. PCMS-DCMI, 23 r. du Loess, 67034 Strasbourg, Fr.

E-mail: ovidiu.pana@itim-cj.ro

Abstract. Charge transfer across interfaces is a fundamental process underpinning a wide range of phenomena, from electrochemistry and catalysis to semiconductor device operation and biological electron transport. A critical aspect of this process is the evanescent tail of electronic wavefunctions, which enables quantum tunneling by allowing a non-zero probability for electrons to traverse potential barriers. The efficiency of this tunneling is strongly influenced by the availability of electronic states—particularly defect states—near the interface, which can serve as resonant pathways that facilitate enhanced electron transfer. Hybrid systems combining half-metals and transition metal dichalcogenides (TMDs) offer tunable properties resulting from interfacial coupling and dimensionality-driven proximity effects. Among TMDs, layered MoS_2 thin films with induced ferromagnetism are especially promising for spintronic applications. Magnetic proximity effects—where the magnetic properties of a non-magnetic material are influenced by an adjacent ferromagnet—play a key role in such systems. In this work, $L1_0$-ordered FePt half-metal thin films were deposited on MgO substrates via pulsed laser deposition (PLD) at 700 °C and subsequently coated with MoS_2 films of varying thicknesses. The interface-driven ferromagnetic coupling between FePt and MoS_2 is attributed to a double exchange mechanism, enabled by the alignment of their respective energy bands. As a result, the MoS_2 layers acquire ferromagnetic characteristics and couple magnetically to the underlying half-metal. The heterostructures were characterized using XRD, XPS, UPS and electron microscopy to assess their structural, chemical, and morphological properties. Their magnetic and electronic behaviors were investigated via magnetometry and spin/charge transport measurements, with a focus on elucidating the role of spin-polarized charge transfer at the interface.

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Poster T4-26

Tartrazine, ciprofloxacin and acetamiprid removal from aqueous solutions using modified mica surfaces as adsorbents

S Pintea, I Lung, A Stegarescu, O Opriș, M Mihet, A Turza, S Tripon and M L Soran

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

E-mail: stelian.pintea@itim-cj.ro

Abstract. Mica powder was treated with two different oxides in order to enhance its adsorbing properties towards three classes of pollutants. For this reason, the mica surface was first modified with copper oxide and, subsequently, with iron oxide (MCF). A second combination involved the treatment applied to the mica powder surface using manganese oxide followed by copper oxide (MMC). Both samples were characterized using X-ray diffraction (XRD), Brunauer-Emmett-Teller (BET), Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDX) and Fourier Transformed Infrared Spectroscopy (FTIR) methods. The prepared adsorbent materials were tested for the removal of tartrazine, ciprofloxacin and acetamiprid from synthetic aqueous solutions. While the MCF sample showed promising removal efficiency in the case of tartrazine, there were limited efficiencies in the case of other samples and pollutants.

Poster T4-27

Systematic Hamiltonian construction of multi-Loop Fluxonium qubits

L-M Pioras-Timbolmas[1,2], L Mathe [1] and L P Zarbo[1]

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

[2] Babes-Bolyai University, 1 Mihail Kogălniceanu, 400347, Cluj-Napoca, Romania

E-mail: larisa.timbolmas@itim-cj.ro

Abstract. We present a systematic method for deriving and quantizing the Hamiltonian of a multi-loop superconducting circuit based on the fluxonium architecture. The circuit consists of n Josephson junctions and n+1 loops, each controlled by an external flux. A key feature is the inductive coupling between the readout resonator and the qubit via a shared superinductance. Using the minimum spanning tree approach, we define independent flux variables and derive the loop equations. The Lagrangian is constructed using node and branch variables, then transformed into matrix form. External flux contributions are absorbed through coordinate shifts, simplifying the potential energy. A normal mode decomposition diagonalizes the kinetic term and yields effective circuit parameters. The quantized Hamiltonian includes both linear and nonlinear components, enabling simulation of the system's energy spectrum. This framework unifies and extends existing models such as fluxonium and gradiometric fluxonium.

Poster T4-28

Electrochemical detection of catechol by linear voltammetry using a graphene modified electrode

F Pogacean, L Magerusan, A Turza and S Pruneanu

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

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

Abstract. A graphene sample (EGr) was obtained in a single-step synthesis by electrochemical exfoliation of graphite rods. A combination of 0.05 M ammonium sulfate and 0.05 M ammonium thiocyanate was employed, leading to a graphene sample composed of few-layer, multi-layer and graphene oxide flakes. Due to the mild exfoliation conditions, large sheets with linear sizes in the range of tens to hundreds of micrometers were produced. The LSV technique gave information about the effect of catechol concentration on the electrochemical signal of bare and graphene-modified electrodes. Based on the resulting calibration plots, the corresponding analytical parameters (linear range, sensitivity, limit of quantification and limit of detection) were calculated for each electrode. In the case of the EGr/GC electrode the linear range was from 6×10^{-7} to 1×10^{-4} M catechol. The detection limit was low (1.82×10^{-7} M) while the quantification limit was 6×10^{-7} M. The sensitivity was five times higher than that corresponding to bare GC, proving the excellent electro-catalytic properties of the graphene-modified electrode. The practical applicability of the graphene-modified electrode was tested in tap water, obtaining an excellent recovery of 102%.

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Poster T4-29

Defective C doped ZnO with enhanced photocatalytic and supercapacitor performances

A Popa[1], M Stefan[1], D Toloman[1], A Ammar Uddin[1], B S Vasile[2,3], I Perhaita[4], A Rostas[1] and S Macavei[1]

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

[2] Research Center for Advanced Materials, Products and Processes, National University of Science and Technology POLITEHNICA Bucharest, 060042 Bucharest

[3] Academy of Romanian Scientists, 050045 Bucharest, Romania

[4] Raluca Ripan Institute for Research in Chemistry, Babes-Bolyai University, 30 Fântânele,400294 Cluj-Napoca, Romania

E-mail: adriana.popa@itim-cj.ro

Abstract. Among oxides of transition metals, ZnO gained interest as material applied in photocatalytic and supercapacitor applications due to its excellent electrical conductivity, lower cost, high surface area, and its versatility from the point of view of synthesis method. The present work investigates the influence of defect states on the supercapacitor performance of ZnO and its ability to degrade pollutants from water. The defect density in ZnO was modified by doping with various carbon concentrations. The defect's center evolution was studied by EPR and PL spectroscopy. The photocatalytic activity was tested against two pollutants, Rhodamine B (RhB) dye and oxytetracycline (OTC) antibiotic, under visible light irradiation. A doping degree of 1% C assures the best photocatalytic activity of ZnO nanoparticles, 80% for RhB, and 50% for OTC. The photodegradation mechanism was identified based on the evidence of ROS species generated. Moreover, the same sample exhibits the best electrochemical properties when tested in a symmetric supercapacitor device, showing a maximum specific capacitance of 104.16 F/g at 2 mV/s scan rate with an energy density of 14.46 Wh/kg and excellent cyclic stability. These results demonstrate the versatility of ZnO:C, which can be successfully used in environmental and energy storage applications.

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Poster T4-30

Electrochemical strategy based on graphene-modified electrodes for enhanced ciprofloxacin sensing

S Pruneanu, F Pogacean, L Magerusan

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

E-mail: stela.pruneanu@itim-cj.ro

Abstract. Increased evidence has documented a direct association between Ciprofloxacin (CFX) intake and significant disruption to the normal functions of connective tissues, leading to severe health conditions (such as tendonitis, tendon rupture and retinal detachment). Additionally, CFX is recognized as a potential emerging pollutant, as it seems to impact both animal and human food chains, resulting in severe health implications. Consequently, there is a compelling need for the precise, swift and selective detection of this fluoroquinolone-class antibiotic. Herein, we present a novel graphene-based electrochemical sensor designed for CFX detection and discuss its practical utility. The graphene material was synthesized using a relatively straightforward and cost-effective approach involving the electrochemical exfoliation of graphite, through a pulsing current, in 0.05 M sodium sulphate (Na_2SO_4), 0.05 M boric acid (H_3BO_3) and 0.05 M sodium chloride (NaCl) solution. The resulting material underwent systematic characterization using scanning electron microscopy/energy dispersive X-ray analysis, X-ray powder diffraction and Raman spectroscopy. Subsequently, it was employed in the fabrication of modified glassy carbon surfaces (EGr/GC). Linear Sweep Voltammetry studies revealed that CFX experiences an irreversible oxidation process on the sensor surface at approximately 1.05 V. Under optimal conditions, the limit of quantification was found to be 0.33×10^{-8} M, with a corresponding limit of detection of 0.1×10^{-8} M. Additionally, the developed sensor's practical suitability was assessed using commercially available pharmaceutical products.

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Poster T4-31

Effect of synthesis method and metal ion type on the thermal conductivity of selected polymer complexes

N Terenti, A Nan, I-V Ganea and T Radu

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

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

Abstract. High thermal conductive polymers are important for various applications, such as flexible electronic devices and batteries. In this work we study the influence of the synthesis method (in solution and mechanochemical) on the thermal conductivity of metal complexes based on poly(benzofurane-*co*-arylacetic acid). Furthermore, the impact of the type of metal ions on the thermal behaviour of these polymeric metal complexes is also analysed. The results obtained demonstrate a significant increase in the thermal conductivity correlated with the metal ion employed, which can be attributed to the decreasing ionic radius and the differences in coordination numbers across the polymeric metal complexes.

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Poster T4-32

TiO_2/g-C_3N_4 photoactive composites

M C Roşu[1], C Socaci[1], D V Cosma[1], A Turza[1], A Urda[1,2] and S C Tripon[1,3]

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

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

[3] Electron Microscopy Center "C. Crăciun", Biology & Geology Faculty, Babeș-Bolyai University, 5-7 Clinicilor, 400006, Cluj-Napoca, Romania

E-mail: marcela.rosu@itim-cj.ro

Abstract. TiO_2/g-C_3N_4 composites were successfully synthesized via hydrothermal method, followed by high-temperature calcination at 700 °C for 1 hour under controlled atmospheres (Ar and Ar/H_2). The resulting materials were characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and UV–visible spectroscopy (UV–Vis) to investigate their morphological, structural, and optical properties. TEM analysis revealed irregularly shaped TiO_2 particles uniformly dispersed on the g-C_3N_4 surface. XRD confirmed the presence of both anatase and rutile crystalline phases of TiO_2. UV–Vis spectra exhibited a red shift in the absorption edge of the TiO_2/g-C_3N_4 composites, indicating bandgap narrowing and an extended photoresponse in the visible region. These findings highlight the potential of TiO_2/g-C_3N_4 composites as promising photoactive materials for visible-light-driven applications.

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Poster T4-33

Bioinspired self-healing microcapsules based on crystalline hydroxyapatite for dental remineralization and repair

M A (Tăut) Stan[1], M Moldovan[2], L Silaghi Dumitrescu[2], A G Paltinean[2], M Filip[2], I Petean[3], I Ardelean[1]

[1] Physics and Chemistry Department, Technical University of Cluj-Napoca, 400394 Cluj-Napoca, Romania; EUT+ Institute of Nanomaterials & Nanotechnologies EUTINN, European University of Technology, European Union.

[2] Raluca Ripan Institute for Research in Chemistry, Babes, -Bolyai University, 30 Fantanele Street,400294 Cluj-Napoca, Romania.

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

E-mail: amalia.taut@chem.utcluj.ro

Abstract. Composite materials used for restorations are prone to microcracks and degradation over time in modern dental treatments. Therefore, there is a growing interest in developing self-healing systems that can extend the lifespan of dental restorations. Although microcapsules (MCs) have been incorporated into dental resins to confer self-healing functionality, their clinical performance remains limited due to the fragility of their organic shells and the restriction to a single healing event during their service life. In our study we synthesized and characterized a novel class of nanoparticle-modified microcapsules featuring a crystalline hydroxyapatite shell, aiming to enhance structural stability and enable multiple self-healing cycles. Microcapsules containing between 0% and 20% hydroxyapatite were synthesized via an in-situ polymerization method. The resulting microcapsules were characterized in terms of their morphology and topography using high resolution SEM and AFM microscopy. The involved chemical bonds were characterized through FTIR and RMN spectroscopy. Our findings clearly show the nano-hydroxyapatite incorporation within micro-capsules slightly increasing the surface roughness, but the efficacy is confirmed by the P-O bonds evidenced by FTIR spectroscopy indicating the activation of self-healing compound. The incorporation of hydroxyapatite not only reinforces the mechanical integrity of the microcapsules but also introduces bioactivity and remineralization potential, making them highly suitable for advanced dental restorative applications.

Poster T4-34

Synthesis of Calcium Phosphate-ZnO composites from natural wastes

M Stan, M Miclaus and S C Tripon

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

E-mail: manuela.stan@itim-cj.ro

Abstract. The synthesis of different types of calcium phosphates, including hydroxyapatite (HAp), from natural biowaste materials rich in calcium has gained considerable interest among researchers. The aims of synthesizing such compounds from natural sources resulted in significant contribution to natural resource management, health care and waste utilization. The combination of various calcium phosphates with metal oxide nanomaterials is an alternative approach to synthesize composites for many applications. Hydroxyapatite is a widely used ceramic biomaterial. In this work, composite particles based on ZnO and calcium phosphates derived from natural biowastes (e.g. snail shells), were obtained by chemical precipitation and calcination method. The crystallinity, morphology and presence of chemical elements were studied by XRD (X-ray diffraction), SEM (scanning electron microscopy), TEM (transmission electron microscopy) and EDS (energy dispersive spectroscopy).

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Poster T4-35

Photocatalytic properties of office paper waste derived activated carbon for efficient degradation of organic pollutants

M Stefan, D Toloman, A Popa, C Leostean, A Varadi, I Perhaita, M Dan, A Rostas, S Tripon and S Macavei

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

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

Abstract. Sustainable waste recycling continues to be one of the most significant challenges in this century, especially for the office paper sector. On top of that, photocatalysis depends on solar radiation as an unlimited and environmentally friendly energy source for removing organic pollutants from contaminated water. The obtaining of activated carbon (AC) from office paper waste was carried out with the help of the chemical activation method using $ZnCl_2$ as an activation agent, followed by heating the samples in adequate conditions. In the present research, we assessed the influence of the amount of $ZnCl_2$ activator on the properties of AC. In our experimental conditions, a part of $ZnCl_2$ was transformed into ZnO, deposited onto AC, and formed a composite. We attempted to minimize aggressive chemical agents through inexpensive technical solutions and experimental approaches. The properties of the obtained AC samples were evaluated by XRD, XPS, SEM/EDX, EPR, and surface area and porosity investigations. All of the samples exhibit photocatalytic activity toward Rhodamine B (RhB). The photocatalytic mechanism was evaluated considering the existence of reactive oxygen species (ROS), evidenced by spin-trapping experiments.

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Poster T4-36

New materials based on biochar and metal oxides. Preliminary depollution tests

A Stegarescu[1], I Lung[1], O Opriş[1], M Miheţ[1], I Kacso[1], A Turza[1], S Tripon[1], M L Soran[1], A Ghendov-Moşanu[2], R Sturza[2]

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

[2] Faculty of Food Technology, Technical University of Moldova, 168 Ștefan cel Mare Str., MD 2004, Chișinău, Republic of Moldova

E-mail: adina.stegarescu@itim-cj.ro

Abstract. Water pollution with pharmaceutical or dyes compounds represents a significant concern for both human health and the environment. Using waste biomass for obtaining biochar as an adsorbent for removing pollutants from contaminated water is a promising solution due to their ability to adsorb organic pollutants from the environment. The relatively low production costs, the widely available wastes have directed the attention of the scientist towards the use of biochar, either in their raw or functionalized/modified version, as a possible solution for the increasing pollution of freshwater sources. Adsorption is considered the most effective method for removing organic pollutants from both water and terrestrial environments.

This paper is foccus on the preparation and characterization of cost-effective new adsorbent materials based on biochar functionalized with metal oxides (Fe_3O_4 and NiO), and preliminary tests for pollutant retention (paracetamol and tartrazine) from water. The obtained materials were characterized by transmission/scanning electron microscopy (T/SEM), energy dispersive spectroscopy (EDX), Brunauer-Emmett-Teller (BET) analysis, Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) analysis.

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Poster T4-37

Sorption capacity of phthalate residues on biochar obtained from apple waste and functionalized with metal oxides

M L Soran[1], O Opriș[1], I Lung[1], S Tripon[1], A Turza[1], I Kacso[1], M D Lazar[1], M La Pietra[2,3], R Truffa[2,3], R Sturza[4], A Ghendov-Mosanu[4], D Lazacovici[4], Y Dasgan[5], M Militaru[6], A Stegarescu[1] and S Bellucci[2,7]

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania
[2] INFN—National Laboratories of Frascati, Via Enrico Fermi 54, 00044 Frascati, Italy
[3] H1 SRL, Via Emanuele Gianturco 6, 00196, Rome, Italy
[4] R.A.I.T. 88 S.R.L, Via Pieve Torina, 64/66, 00156 Rome, Italy
[5] University of Cukurova, Balcali, 01330 Balcali, Adana, Türkiye
[6] Research Institute for Fruit Growing, Marului, 402, Maracineni 117450, Arges Romania
[7] R.A.I.T. 88 S.R.L, Via Pieve Torina, 64/66, 00156 Roma, Italy

E-mail: rodica.sturza@chim.utm.md

Abstract. The Water Framework Directive includes phthalates in the list of priority and ubiquitous contaminants. The present study focused on characterizing the sorption capacity of biochar obtained from apple waste for phthalate residues – di-butyl (DBP) and bis(2-ethylhexyl)phthalate (DEHP) from water. The sorption activity was tested on 7 experimental samples of functionalized biochar. Several series of experiments were performed: (1) determination of the biochar sorption capacity ($\overline{A}$, µmol/g) as a function of pH (3-9); (2) establishment of adsorption isotherms at three temperatures (288 K, 298 K and 308 K) and (3) adsorption kinetics at pH 7. Phthalate concentrations were determined chromatographically - GCMS-QP-2010S (IS), on a Restek - Rtx-5MS silica column (30 m/0.25 mm/0.25 µm 5% diphenyl phase / 95% dimethylpolysiloxane. In the study of adsorption kinetics, tests were performed at equal time intervals (30 min). Langmuir and Freundlich models, pseudo-first and second order kinetic models were used to analyze the experimental data.

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Poster T4-38

Influence of anatase / rutile proportion on the tribological performance of engine oils

R C Suciu[1], A Molea[2], **I Barabás[2] , M Cioaza[3], C Bîrleanu[3]**

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

[2] Department of Automotive and Transport Engineering, Technical University of Cluj-Napoca, 103-105 Muncii Bd., 400641 Cluj-Napoca, Romania

[3] Department of Mechanical Systems Engineering, Technical University of Cluj-Napoca, 103-105 Muncii Bd., 400641 Cluj-Napoca, Romania

E-mail: Ramona.Suciu@itim-cj.ro

Abstract. The traditional lubrication additives cannot satisfy the needs of machinery and equipment and produce toxic soot nanoparticles rich in sulphur and phosphorus harmful to environment and human health. This inconvenient can be reduce using nanoparticles because they can easily enter the friction contact zone to keep of the rubbed metal surfaces and greatly improve the tribological properties of lubricants. The investigation aims to determine the optimal proportion of anatase / rutile of nanoaditives dispersed in 10W – 40 pure base engine oil. The nanoaditives were preparing via wet – chemical techniques, using Titania P25, bi-distilled water, acetylacetone and Triton X as surfactant. The samples were heat – treated hour at 450 - 750°C. DTA – TG – DTG, X–ray diffraction, FT – IR, UV – Vis, Raman spectroscopies, SEM and TEM were assessed to investigate the thermal, structural, optical and morphological properties. The stability investigation were carried out by comparing absorbance condition using UV – VIS spectrophotometer at each anatase / rutile proportion. The tribological test were performed at 40°C using a four ball tribometer under standardized load and speed conditions. Key tribological parameters—coefficient of friction, wear scar diameter, and extreme pressure performance—were measured to evaluate the lubricant's effectiveness. Results indicate that the anatase/rutile proportion significantly influences the tribological response, with specific ratios exhibiting superior anti-wear and friction-reduction properties. These improvements are attributed to the formation of stable, adherent tribofilms and the rolling and mending effects of the nanoparticles under boundary lubrication conditions.

The findings provide valuable insights into the optimization of nanoparticle-based additives in lubricants, highlighting the critical role of TiO_2 polymorphic composition in enhancing tribological performance while promoting environmentally friendly lubrication strategies.

Poster T4-39

Optimization and scaling-up strategies of synthesis of poly(tartaric acid) for future industrial applications

N Terenti[1], A Bunge[1], I Rigo[2] and A Nan[1]

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

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

E-mail: natalia.terenri@itim-cj.ro

Abstract. Scaling up polymerisation reactions is a critical process in the chemical industry, enabling the transition from laboratory-scale experiments to large-scale industrial production. This whole process includes finding the optimal parameters between the chemistry, properties and economic factors and most of the time it requires interdisciplinary collaboration. Herein we present our progress from synthesis of poly(tartaric acid) to optimizing of the reactions at different quantities and scaling-up to five hundred grams. Poly(tartaric acid) is a relatively new polymer synthesized by our group from a biologically produced precursor – tartaric acid, using a simple thermal treatment without need for the use of solvents or catalysts. The obtained result show that the adsorption bands attributed to carboxylic and hydroxyl groups in the 13C ss-NMR and FTIR spectra did not undergo significant changes when the reaction was scaled up from 5 g to 500 g. Furthermore, the thermal properties of polymers, as determined by TGA, thermal conductivity, and thermal diffusivity, highlighted the successful upscaling process. These findings validate the robustness of the polymerization methodology, demonstrating its scalability while preserving chemical integrity.

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Poster T4-40

gC_3N_4 decorated with ZnO:Mn rods for enhanced photocatalytic performance

D Toloman, M Stefan, S Macavei, L Barbu-Tudoran, A Popa

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

E-mail: dana.toloman@itim-cj.ro

Abstract. In the present research, ZnO:Mn rods obtained from recycled anodic paste of spent Zn-MnO_2 alkaline batteries were immobilized on the surface of gC_3N_4 and tested as photocatalysts for degradation of Rhodamine B (RhB) under visible light irradiation. The effects of the ratio between the two components of the composite materials on the RhB removal rate was investigated. The successful achievement of the composite material was proved by X-ray diffraction (XRD), Scanning transmission electron microscopy (STEM), Fourier Transform Infrared Spectroscopy (FTIR) and electron paramagnetic resonance (EPR). The composite samples show enhanced photocatalytic activity under visible irradiation compared with ZnO:Mn. The sample with the ration 1-0.1 between gC_3N_4 and ZnO:Mn has the highest removal rate of 93% and the superoxide radicals are the reactive oxygen species involved in dye degradation as evidence by EPR spectroscopy coupled with the spin trapping technique. The coupling between gC_3N_4 and ZnO:Mn suppress the electron-hole pairs recombination, improving the photocatalytic performance. The best photocatalytic kinetic constant being almost six time higher than in the case of ZnO:Mn. Moreover, the sample have a good stability, the removal rate was slightly modified after 5 consecutive reaction cycles.

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Poster T4-41

Gold-decorated titania nanotubes with graphene for visible light-mediated amoxicillin photodegradation

A Urda[1,2], D Lazar[1], D Cosma[1], I Grosu[2] and C Socaci[1]

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

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

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

Abstract. This study explores the development of advanced photocatalysts based on titanium dioxide (TiO_2) nanotubes combined with gold nanoparticles and graphene materials. Two types of graphene derivatives (reduced graphene oxide and nitrogen-doped graphene) were incorporated to improve the catalysts' properties. The materials were thoroughly analyzed to confirm their structure and composition. Tests showed that the presence of graphene enhanced the catalysts' ability to absorb visible light, which is important for using sunlight effectively. Among the tested samples, the catalyst containing nitrogen-doped graphene showed the best performance, breaking down up to 60% of the antibiotic amoxicillin under visible light. The degradation process followed predictable kinetics, indicating efficient photocatalytic activity. The improved performance is explained by better separation of electrical charges and increased light absorption due to the graphene modifications. These results suggest that combining TiO_2 nanotubes with gold and graphene materials can lead to effective solutions for removing antibiotic pollutants from water using solar energy.

Poster T4-42

Study on the influence of hybrid gold-iron oxide nanoparticle shape on the in vivo hepatotoxicity

A Vădan[1,2], A Stoica[2,3], S Toth[1,2], A Ciorîță[2,3], R Marica[4], C Dobre[2], F Arik[5], S Klein[5,6], S Boca[3,7]

[1]Doctoral School of Integrative Biology, Faculty of Biology and Geology, Babes-Bolyai University, 400015 Cluj-Napoca, Romania
[2]Department of Molecular Biology and Biotechnology, Faculty of Biology and Geology, Babes-Bolyai University, 400015 Cluj-Napoca, Romania
[3]National Institute for Research and Development of Isotopic and Molecular Technologies, 400293 Cluj-Napoca, Romania
[4]Faculty of Veterinary Medicine, University of Agricultural Sciences and Veterinary Medicine, 400372 Cluj-Napoca, Romania
[5]M3 Research Center, University Clinic Tübingen, D-72076 Tübingen, Germany
[6]Physical Chemistry I, Department of Chemistry and Pharmacy, Friedrich-Alexander University Erlangen-Nürnberg, 91058 Erlangen, Germany
[7]Interdisciplinary Research Institute in Bio-Nano-Sciences, Babes-Bolyai University, 400271 Cluj-Napoca, Romania

E-mail: sanda.boca@itim-cj.ro

Abstract. Hybrid gold-iron oxide nanoparticles (Au-Fe3O4 NPs) have gained increasing interest in biomedical applications due to their multifunctional capabilities. Although attractive, such nanoparticles can trigger toxicity in healthy tissues. Hence, a comprehensive toxicological examination is required to ensure their general safety. In this study, flower and dumbbell shaped Au-Fe3O4 NPs were administered on female Wistar rats over a period of 14 days by using varied dosing regimens at different time intervals. Markers of membrane integrity, oxidative stress indicators, iron concentration, histopathology and electronic microscopy images of rat liver were analysed. The results indicate a depletion of the antioxidant pool in the blood plasma. An activation of the antioxidant defence mechanisms against reactive oxygen species was observed in the liver. However, the changes in enzyme levels as markers of cellular damage and the histopathological examinations indicate no obvious hepatocellular alterations. The biochemical, histological and ultrastructural data clearly indicate an influence related to the particle shape, dumbbells inducing transient changes in plasma and liver, while nanoflowers causing greater plasma redox imbalance.

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Poster T4-43

Synthesis and characterization of nanocomposites based on GO/rGO and Li doped ZnO for supercapcitor application

A Varadi[1,2], M Stefan[1], D Toloman[1], A Popa[1], A Rostas[1], D Lazar[1], C Leostean[1], S Macavei[1], A Ammar[1], E Erdem[1,3]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
[2]Doctoral School of Chemistry, Babes-Bolyai University, Cluj-Napoca, Romania
[3]Faculty of Engineering and Natural Sciences, Sabanci University, Istanbul, Turkey

E-mail: ana.varadi@itim-cj.ro

Abstract. Graphene oxide (GO) and reduced graphene oxide (rGO) have been widely studied for various applications due to their good physicochemical properties such as large surface area, chemical stability and excellent electrical conductivity. In this work, we have synthesized GO(rGO)-ZnO:0.5%Li nanocomposites in 3 weight ratios: 1:1, 1:0.5 and 1:2, using the nano-rods morphology for 0.5% Li doped ZnO. The nanocomposites samples were characterized by XRD, SEM/TEM and PL, UV-Vis, Raman and EPR spectrometry. The samples were also tested as electrode material for supercapacitor application. GO-ZnO:0.5%Li sample having weight ratio 1:1 showed the highest specific capacitance value at each scan rate, compared to the other two devices, highlighting its superior electrochemical performance. This sample exhibited the longest discharge time. The cyclic stability of the devices was tested and the best performing device presented a retention of about 85% after 500 cycles.

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Poster T4-44

Studies on g-C_3N_4-TiO_2:Mn based nanocomposites with photocatalytic properties

M Stefan[1], D Toloman[1], A Popa[1], C Leostean[1], A Varadi[1], M Groza[1], R Nastas[2], S Tripon[1], S Macavei[1]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
[2]Institute of Chemistry, State University of Moldova, 3 Academiei St, M2028 Chisinau, Republic of Moldova

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

Abstract. Nanocomposites based on graphitic carbon nitride are receiving considerable interest in the field of science due to their unique properties, such as their facile synthesis, versatility, robustness under extreme conditions, and remarkable chemical durability. Additionally, nanocomposites made up of two or more components exhibit new physicochemical features assembled in a single entity that can be used in a variety of engineering applications. The present work reveals our results regarding synthesis and characterization of g-C_3N_4-TiO_2 :Mn nanocomposites with photocatalytic properties. A simple and cost-effective method for g-C3N4 synthesis is represented by the thermal polycondensation of urea and/or melamine. On the other hand, TiO_2:Mn nanoparticles were prepared through a sol-gel process and the g-C_3N_4-TiO_2:Mn nanocomposites were assembled from two individual components by using the linking polymer polyallylamine hydrochloride (PAH). The properties of the obtained samples were evaluated by XRD, XPS, SEM/EDX, EPR, and surface area and porosity investigations. All of the samples exhibit photocatalytic activity toward Rhodamine B (RhB). The proposed photocatalytic mechanism was evaluated considering the existence of reactive oxygen species (ROS), evidenced by spin-trapping experiments.

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SPECIAL STUDENT SECTION

Poster S-1

Half-metallic compensated ferrimagnetism in the $Co_{0.5}Mn_{1.5}Al$ half-Heusler compound: experimental and theoretical investigations

E Bender[1], R Hirian[1], S Macavei[2], C Leostean[2], S Gutoiu[2], L Barbu-Tudoran[2], D Benea[1]

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

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

E-mail: diana.benea@ubbcluj.ro

Abstract. Theoretical and experimental investigations on the electronic and magnetic properties of the $Co_{0.5}Mn_{1.5}Al$ half-Heusler compound are presented. This material has been reported as a half-metallic fully compensated ferrimagnet (HMFi), with potential usage in spintronic devices. Experimental results indicate ferrimagnetic behavior that is nearly fully compensated, with a saturation magnetization of 0.09 μ_B/f.u. for the $Co_{0.5}Mn_{1.5}Al$ samples. This result is in agreement with previous reports, which slightly contradicts the Slater-Pauling rule. Magnetization versus temperature measurements found a Curie temperature of 670 K. The analysis of the X-ray diffraction (XRD) pattern was employed to identify the type of disorder in the sample. The electronic band structure calculations using the Korringa-Kohn-Rostoker (KKR) Green's function method have been performed to investigate the impact of substitutional disorder on half-metallicity and the ferrimagnetic compensation. These studies explore the underlying mechanisms that contribute to the alloys unique electronic structure and magnetic behavior. Understanding these properties could lead to significant advancements in the development of efficient spintronic applications.

Poster S-2

Superconducting Thin Films Fabricated Using the Sol-Gel Spin Coating Method

A Mateaş[1] and C Tiușan[1,2]

[1] Babeș-Bolyai University, Faculty of Physics, Mihail Kogălniceanu Street, Cluj-Napoca, Romania
[2] National Centre for Scientific Research, 54000, Nancy, France

E-mail: adrianmateas10@gmail.com, adrian.mateas@stud.ubbcluj.ro

Abstract. Since the discovery of $Bi_2Sr_2Ca_{n-1}Cu_nO_\delta$ (BSCCO), it has been researched extensively, due to its desired properties: superconductivity and the high transition temperature (Tc). From the high-performance, low-cost and large-scale industrialization perspective, chemical methods are more suitable for fabricating BSCCO thin films. Compared with other methods, the Sol-Gel technique has many advantages such as low cost, high efficiency, easy handling, molecular level homogeneity, lower sintering temperatures and overall diminished energy consumption. A stable and homogeneous gel was formed by employing a modified Pechini sol-gel method which uses nitrate salts, ethylenediaminetetraacetic acid and ethylene glycol to create the desired gel. The manufacturing of thin films involved implementing the spin coating technique to deposit our precursor gel on to substrates followed by thermal treatment. In this study Bi-2212 superconducting thin films were fabricated by the sol-gel spin coating method and related characteristics have been investigated.

Poster S-3

Exploring Romanian archaeological ceramics via solid-state NMR spectroscopy

R G Stroia[1], M Vasilescu[1], S M Herlea[2], A M RGherman[3], L Barbu[3,4], C Filip[3], and A Simion[1,3]

[1]Faculty of Physics, Babes-Bolyai University, 400084 Cluj-Napoca, Romania
[2]Faculty of Social Sciences and Humanities, Lucian Blaga University, 550024 Sibiu, Romania
[3]National Institute for Research and Development of Isotopic and Molecular Technologies 400293 Cluj-Napoca, Romania
[4]Faculty of Biology and Geology, Babes-Bolyai University, 400015 Cluj-Napoca, Romania

Abstract. Archaeological ceramics provide vital insights into past human societies, offering information about daily life, trade, technology, and cultural practices. In this study, we employ nuclear magnetic resonance (NMR) spectroscopy to analyze the molecular and structural properties of three ceramic samples from archaeological sites in Romania: Capidava, the Dacian Fortress of Tilișca, and Șura Mică. These artifacts span the Pre-Roman, Dacian (9th century BC – 2nd century AD), and Early Medieval (9th–11th century AD) periods. Using magic-angle spinning (MAS) NMR for ^{1}H, ^{27}Al, ^{29}Si, and ^{31}P nuclei, alongside electron microscopy, we characterize materials from both surface and inner ceramic layers. The ^{1}H spectra indicate porosity variations; ^{29}Si results reveal differing silica environments (Q^3/Q^4) linked to firing techniques; ^{27}Al spectra suggest distinct aluminum coordination patterns, with Șura Mică samples showing a balanced composition; and ^{31}P signals reflect diverse phosphorus environments. These findings reveal technological contrasts: Roman-era ceramics show refined production, Dacian pieces retain traditional methods, and Early Medieval samples emphasize utilitarian function over durability.

Poster S-4

Plasmonic Calligraphy: A portable multiplex nanosensor for ultrasensitive and multimodal biomolecule detection

D Ursa[1,2], D Stoia[1,2], M Lamy de la Chapelle[3], M Focșan[1,2]

[1]Nanobiophotonics and Laser Microspectroscopy Centre, Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, 42 T. Laurian Street, 400271, Cluj-Napoca, Romania

[2]Biomolecular Physics Department, Faculty of Physics, Babes-Bolyai University, 1 M. Kogalniceanu Street, 400084, Cluj-Napoca, Romania

[3]IMMM – UMR 6283 CNRS, Le Mans Université, Olivier Messiaen Avenue, 72085 Le Mans, France

E-mail: daria.ursa@stud.ubbcluj.ro

Abstract. Nanobiophotonics, an interdisciplinary field at the intersection of nanotechnology, biology, and photonics, enables the manipulation and detection of biomolecular interactions at the nanoscale using light, offering powerful tools for biomedical sensing and diagnostics. The innovative concept of the proposed nanotechnology relies on the implementation of the plasmonic calligraphy approach for creating well-isolated plasmonic regions onto a paper support, thus obtaining a well-desired multiplexing capability of the sensors. As plasmonic inks, efficient gold nanoparticles previously synthesized in different shapes were functionalized with sequence-specific oligonucleotides, specifically polyadenine (Poly A). The as-caligraphed active lines allows ultrasensitive, label-free detection of complementary poly-thymine (Poly T) sequences via both Surface-enhanced Raman spectroscopy (SERS) and thermoplasmonic sensing. Its portability enables on-site validation of the personalized, paper-based plasmonic sensor under controlled conditions. Operating without molecular labeling, the device is compatible with real-time diagnostic applications. These findings highlight the potential of plasmonic calligraphy as a powerful tool for advanced biomedical analysis.

AUTHOR INDEX

A

B

C

D

E

F

G

H

I

J

K

L

M

N

U

V

W

Z

Zagrai M - Poster T3-2, Poster T3-5, Poster T3-8, Poster T3-14, Poster T4-11
Zani V - Poster T2-4
Zarbo L P - Oral T3-6, Poster T3-6, Poster T4-27
Zavkibekova K - Oral T4-11
Zhuravskii S - Poster T2-22
Zikaria K - Poster T2-8