



13th International Conference  Physics of
4th Autumn School  Advanced Materials

Abstract Book ICPAM-13



September 24 - 30, 2021

San Feliu de Guixols, Spain

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ICPAM-13

**12th International Conference on Physics of
Advanced Materials**

**September 24-30, 2021, Sant Feliu de Guixols, Spain
www.icpam.ro**

Daily Program and Abstracts

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Cover: Laura Velicu, Dragos Dutu



Foreword

The 13th International Conference on Physics of Advanced Materials (ICPAM-13) continues the tradition of the previous conferences organized by the Faculty of Physics of Alexandru Ioan Cuza University of Iasi at every four years, since 1980, and at every two years since 2012.

Beginning with 2012, the conference has as co-organizers prestigious institutions. Due to their contribution, the scientific quality of the conference increased, the conference papers being published in special issues in *Materials Science and Engineering: B*; *Applied Surface Science*, *Thin Solid Films* and *Material Today: Proceedings*.

In 2014 the first autumn school on Physics of Advanced Materials, PAMS-1 was held in parallel with ICPAM-10. This event is focused on providing interdisciplinary expert training, involving both fundamental knowledge and current research topics. The fact that the school is organized in parallel with the conference assures a better interaction between the conference participants involved in different fields of physics of advanced materials and the participants attending the school. In the same year we began the collaboration with the 4th International Festival of NanoArt, promoting the art and science interaction.

Since 2016, beginning with ICPAM-11, the conference and the events hosted by the conference became itinerant.

For the first time, the 13th edition, the 4th Autumn School on Physics of Advanced Materials (PAMS-4), and the 5th

International Festival of NanoArt are organized in a hybrid form.

Over 180 participants contributed with around 200 abstracts (ICPAM-13 and PAMS-4) for plenary, invited, oral and poster presentations.

We invite participants to publish their results, presented in the conference, in the special issues of Thin Solid Films, Coatings, Materials and Nanomaterials journals. These journals are partners and sponsors at the same time, sustaining the conference and the autumn school.

The special Issues are:

Advanced Thin Films and Nanostructures -Selected papers from ICPAM-13, Sant Feliu de Guixols, 2021-AFN-ICPAM-13 published by Thin Solid Films

New trends in Functional Materials and Devices, published by Coatings

New developments in physics of advanced materials, published by Materials

New Achievements in Nanostructured and Low Dimensional Materials and Systems, published by Nanomaterials.

Manuscripts should follow the instructions and the deadlines given on <https://icpam.ro/papers-publication/> .

We would like to thank all participants for their important scientific contribution and the sponsors and partners for their support.

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Conference topics and topics chairpersons

T 1: Thin Films and Nanostructures for Modern Electronics

Daniel MORARU, Shizuoka University, Japan

Abdullah YILDIZ, Ankara Yıldırım Beyazıt University

T 2: Fundamentals of Plasma and Laser-Material Interactions
and Processing

Cristian FOCSA, Université des Sciences et Technologies de Lille

T 3: Materials for Energy and Environment

Silviu COLIS, University of Strasbourg

Viaceslav BARSUKOV, Kyiv National University of Technologies
and Design

T 4: Magnetic Materials, Spintronics and Related Devices

Coriolan TIUSAN, Technical University Cluj-Napoca

T 5: New developments in sensing materials and sensor devices
Firuta BORZA, National Institute of research and Development
for Technical Physics, Iasi

Emmanuel KOUDOUMAS, Hellenic Mediterranean University,
Heraklion

T 6: Nanostructures and Low Dimensional Systems
Isabelle BERBEZIER, University Paul Cézanne, Marseille

T 7: Emerging Electronic Memory Materials and Devices
Shashi PAUL, De Montfort University, Leicester

T 8: Polymer Materials and Composites
Valeria HARABAGIU, Petru Poni Institute of Macromolecular
Chemistry, Iasi

T 9: Biomaterials and Healthcare Applications
Simion SIMON, Babes – Bolyai University Cluj-Napoca
Norbert KUCERKA, Joint Institute for Nuclear Research, Dubna

T 10: Functional Materials. Processing and Characterization
Nikita BITYURIN, Russian Academy of Sciences, Russia Nizhniy
Novgorod

T 11: Self-assembly and Patterning
Joerg K. N. LINDNER, Paderborn University

T 12: Art, Science and Technology
Cris ORFESCU, NanoArt 21, Los Angeles

T 13: Trends in Condensed Matter Theory
Liviu CHIONCEL, Augsburg University

T14: Advanced photonic materials and devices
Dana CRISTEA, National Institute for Research and
Development in Microtechnologies, Bucharest,
Crina COJOCARU, Polytechnic University of Catalonia, Barcelona

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Friday, September 24, 2021

Hotel Eden Rock, Sant Feliu de Guixols

Salon Mediterraneo -HALL 1

16:00 Venue & Registration

18:00 Welcome Cocktail & Nanoart Vernisage

20:00 Dinner

Saturday, September 25, 2021

08:00	Registration
08:20	Opening HALL 1-Salon Mediteraneo
09:10	Plenary Session HALL 1
10:20	Coffee break
11:00	Plenary Session HALL 1
13:20	Lunch
15:00	Plenary, Invited and Oral Sessions HALL 1
18:05	Coffee break & Poster session I HALL 1
	Poster Session I -Online

20:00 Dinner

HALL 1 - 09:10

T4-PL: Voltage-driven ion-migration in magnetic materials: a new approach to enhance energy efficiency

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Electric-field-controlled magnetism could represent a significant breakthrough in the pursuit for new strategies to enhance energy efficiency in magnetically actuated devices. Here I will first report on electrolyte-gated and defect-mediated ionic transport in Co_3O_4 films which allows for room-temperature voltage-controlled ON-OFF ferromagnetism via internal reduction/oxidation processes. Negative voltages partially reduce Co_3O_4 to Co (ferromagnetism: ON), resulting in graded films including Co- and O-rich areas [1]. Positive bias oxidizes Co back to Co_3O_4 (paramagnetism: OFF). This electric-field-induced atomic-scale reconfiguration process is compositionally, structurally, and magnetically reversible and self-sustained since no oxygen source other than the Co_3O_4 itself is required. We will show that the magneto-ionic effects are largely increased using an electrochemical capacitor configuration instead of placing the electric contacts at the side of the semiconductor (electric-double-layer transistor-like configuration). This is due to a greater uniformity and strength of the electric field in the former case [2]. Finally, I will show that the effects of voltage-driven ion

migration are not restricted only to oxygen ion species, but are in fact even more pronounced in transition metal nitrides (CoN, FeN), where nitrogen diffusion occurs at faster rates and with lower threshold voltages than oxygen ion migration [3].

- [1] A. Quintana et al., ACS Nano, 12 (2018) 10291.
- [2] J. de Rojas et al., Adv. Funct. Mater., 30 (2020) 2003704.
- [3] J. de Rojas et al., Nat. Commun. 11 (2020) 5871.

T10-PL: Resolutions to an issue for achieving high carrier transport ZnO- and In₂O₃-based transparent conductive films

T. Yamamoto¹

¹*Research Institute, Kochi University of Technology, Kochi, Japan*

We have been developing a technology which enables high film-deposition-speed, low temperature of less than 250 °C and low-substrate-damage growth of thin films to tailor electrical, optical and mechanical properties of highly transparent conductive oxide (TCO) films such as *n*-type doped ZnO- and In₂O₃-based films.[1-4] Recently, we reported Ce- and H-codoped In₂O₃ films (ICO:H) with a thickness of 100 nm showing high Hall mobility of 145 cm²/(Vs) with solid-phase crystallization: The films were deposited at a substrate temperature of 150 °C by reactive plasma deposition with direct current arc discharge, subsequently were postannealed at 200 °C for 30 min in air. The above process is a very effective way to transform ICO:H films from amorphous to cubic bixbyite polycrystalline structure. Note that we found reduced residual strain in postannealed ICO:H films compared with polycrystalline ICO:H films obtained by RPD under high vacuum condition. This is a key factor for achieving high carrier

transport TCO films. The successful fabrication is based on two factors: (1) the effective ionic radius of Ce^{4+} with a coordination number of six is close to that of In^{3+} with the same coordination number, leading to the reduction of microstrain in the vicinity of the donor-dopant sites; (2) the amount of oxygen vacancies can be reduced by the use of Ce dopants having high oxygen affinity compared with host In atoms. This improves crystallinity exhibiting long-range lattice order. As a result, we have achieved high Hall mobility In_2O_3 -based TCO films. [1,2]

Concerning ZnO-based polycrystalline TCO films, in light of carrier transport, we have had some issues to be resolved: (1) It is very difficult to realize large grain size to enhance the contribution of grain-boundary carrier scattering on the carrier transport; (2) The use of conventional direct-current magnetron sputtering (DC-MS) produces ZnO-based TCO films showing large-angle-grain-boundary-based columnar structure with a poor preferential (0001) orientation. For a solution to the second issue above, we have proposed the following technology: Firstly 10-nm-thick Ga-doped ZnO films are deposited by RPD as an interface layer, then Al-doped ZnO (AZO) films are deposited on the substrate with the above interface layer by DC-MS. As a result, we have achieved AZO films with a well-defined (0001) orientation showing improved Hall mobility [3,4]

[1] E. Kobayashi, Y. Watabe, and T. Yamamoto, *Appl. Phys. Express*, 8 (2015) pp. 015505-1-015505-4.

[2] E. Kobayashi, Y. Watabe, T. Yamamoto, and Y. Yamada, *Sol. Energ. Mat. Sol. C*, 149 (2016) pp. 75-80.

[3] J. Nomoto, H. Makino, and T. Yamamoto, *Sci. Adv. Mater.*, 9 (2017) pp. 1815-1821.

[4] J. Nomoto, H. Makino, and T. Yamamoto, *Nanoscale Res. Lett.* (2016) 11:320.

Plenary Session

HALL 1 - 11:00

T13-PL: Interplay between surface charge accumulation, conduction band filling and ferroic ordering

Cristian Mihail Teodorescu¹

¹Surfaces and Interfaces, National Institute of Materials Physics, Magurele, Romania

The Heisenberg interaction with the subsequent mean field Curie-Weiss approach predicts too elevated coercive fields for ferromagnetism. Thus, the band theory of ferromagnetism is more appropriate to describe this phenomenon in metals. The drawbacks of this theory is the prediction of too elevated Curie temperatures and the rather ambiguous definition of the energy parameter U which intervenes in the Stoner criterion $Ug(\epsilon_F) > 1$, where $g(\epsilon)$ is the paramagnetic density of states (DOS), and ϵ_F is the Fermi kinetic energy. It is, however, observed that the Stoner theory does not account correctly for total electron energies in the sub-bands with majority and minority spins. By evaluating correctly these energies, one may infer a new criterion for ferromagnetism such as: $(dg/d\epsilon)(\epsilon_F) \int_0^{\epsilon_F} g(\epsilon) d\epsilon < g^2(\epsilon_F)$. In other words, the metal is ferromagnetic in all cases where the DOS has a negative slope

with increasing energies. By introducing crystal field based simplified DOSs, one may predict along the 3d metals the most stable structures, derive which metals in which structures are ferromagnetic, explain the low coercive fields by conservation of the electron number, and predict reasonable Curie temperatures. As a bonus, at very elevated temperatures most metals (if they still exist in the solid state) become again ferromagnetic, which offers an appealing origin for the geomagnetic field [1]. For ferroelectricity in thin films, a new microscopic model is proposed where the stabilization of the ferroelectric state is driven by charge accumulation at the interfaces of the film. This microscopic energy for elemental dipoles in the material may then be treated in the Curie-Weiss model to yield state equations in good agreement with experiments [2]. As a consequence, both ferroelectricity and ferromagnetism in thin films may be related by charge accumulation and band filling. This offers the possibility to engineer new multiferroic heterostructures with electronic coupling between the two phases.

[1] C. M. Teodorescu, Res. Phys. 25 (2021) 104241.

[2] C. M. Teodorescu, Phys. Chem. Chem. Phys. 23 (2021) 4085.

T3-PL: Physical Properties of chalcogenide thin films with or without Cd, used in photovoltaics for terrestrial and space applications

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¹*Department of Electricity, Solid State and Biophysics, Faculty of Physics, University of Bucharest, 077125, Magurele-Ifov, Atomistilor 405, Romania*

Due to their physical and chemical properties (such as suitable band gaps, large absorption coefficients and good chemical stability) the polycrystalline ZnX (X=S, Se, Te) and CdTe thin films, are interesting materials for electronic and optoelectronic devices, including the photovoltaic cells for both terrestrial and space applications. For this specific application, it is of prime importance to study the physical properties of the component thin films prepared by different techniques and the influence of ionizing radiations on their properties.

In this paper, polycrystalline ZnX (X=S, Se, Te) were prepared by rf magnetron sputtering at different RF powers, different deposition times, different working pressures, and characterized to determine the optimal growth conditions for high quality very thin Cd free films, used especially as windows layer in the photovoltaic cells based on the CdTe thin film as main absorber. The CdTe thin films were prepared by thermal vacuum evaporation. Structural properties were studied by X – ray diffraction (XRD) and the crystalline structure parameters were determined by analyzing the samples in Bragg-Brentano theta-theta geometry.

Morphological investigations were made by scanning electron microscopy (SEM) and by atomic force microscopy (AFM). Absorption and transmission measurements were performed in the spectral range between 200 – 1200 nm at room temperature. Thicknesses and band gap energies of the component thin films were determined. The obtained values were between few tens and hundreds nanometers for thicknesses of windows layers and few microns for CdTe films, respectively. The optical band gap was between 2.3 eV and 2.8

eV for window layers and around 1.4 eV for the base absorber CdTe thin film. Electrical measurements were performed on the component thin films and the photovoltaic cells in the dark and at illumination in AM 1.5 conditions. The photovoltaic cells based on ZnX (X= S, Se, Te)/CdTe thin films, were irradiated with protons and alpha particles, (both components of cosmic rays), at room temperature. The irradiation energy for both protons and alpha particles was 3 MeV and the fluencies were 10^{14} protons/cm² and 10^{13} alpha particles/cm², respectively. The effects of irradiation were studied by investigating the changes in the structural, morphological, electrical, and optical properties of the component thin films and prepared cells. The parameters characterizing a photovoltaic cell, short-circuit current, open circuit photo-voltage and fill factor were calculated before and after protons or alpha particles irradiation and the obtained values are compared. A discussion about the possible origin of those defects is given. In this sense, it was found that proton irradiation in the above-mentioned conditions results mainly in the introduction of defects at the CdS/CdTe interface.

- [1] S. Antohe, L. Ion, M. Girtan, O.Toma, Romanian Reports in Physics 65 (2013) 805–811.
- [2] Toma, O.; Ion, L.; Girtan, M.; Antohe, S. Solar Energy, 108 (2014) 51–60. 306 doi: 10.1016/j.solener.2014.06.031.
- [3] O. Toma, L. Ion, S. Iftimie, A. Radu, S. Antohe, Materials & Design, 100 (2016) 198–203, 10.1016/j.matdes.2016.03.117.
- [4] O. Toma, L. Ion, S. Iftimie, V.A Antohe, A. Radu, A. M. Raduta, D. Manica, S. Antohe, Applied Surface Science, 478 (2019) 831–839, doi: 10.1016/j.apsusc.2019.02.032.

[5] L. Ion, S. Iftimie, A. Radu, V. A. Antohe, O. Toma, S. Antohe, Proceedings of the Romanian Academy, Series A, 22 (2021) 25–34.

T6-PL: Femtosecond spectroscopy of excitons and charge carriers in semiconductor quantum dots used in photocatalysis.

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The report is devoted to the study of the dynamics of excitons and charge carriers in quantum dots (QDs) of type II / VI by the method of femtosecond spectroscopy. The talk discusses QDs based on zinc and cadmium chalcogenides, as well as their alloys. Particular attention is paid to QDs doped with Mn or Cu ions. Transient absorption (TA) spectra exhibit the spectral features of excitons and charge carriers. Figure 1. shows transient spectra Mn²⁺ doped QDs.

TA spectra of QDs fabricated from the manganese doped Mn²⁺: Zn_{~0.5}Cd_{~0.5}S/ZnS alloy reveals a specific feature that can be attributed to electrochromic Stark shift of the band-edge exciton. This feature manifests itself as an absorption peak in the TA spectrum appearing at a time delay of about 1 ps. The delayed rising and decay kinetics of this Stark peak in the manganese doped QDs significantly distinguish it from the known Stark peak associated with electrochromic shift caused

by exciton-exciton interactions in undoped QDs at the shortest time delays.

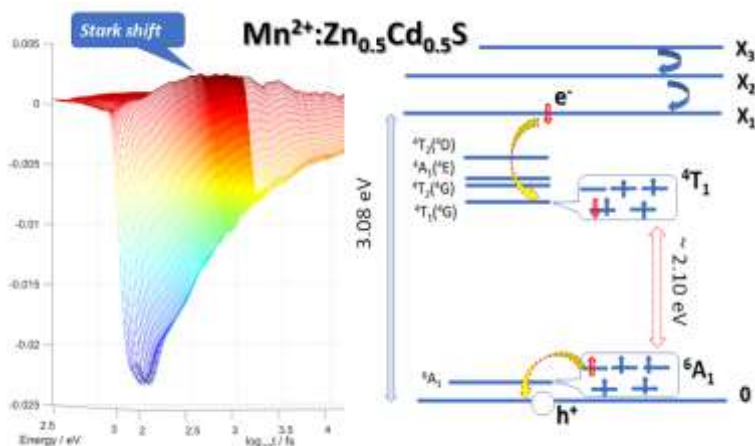


Fig.1 Femtosecond transient absorption spectra of $\text{Mn}^{2+}:\text{Zn}_{0.5}\text{Cd}_{0.5}\text{S}/\text{ZnS}$ QDs (left). Stark peak evidences the charge transfer. Scheme of charge transfer events leading to the Mn^{2+*} excitation (right).

The comparative kinetic analysis of TA spectra of manganese doped and undoped QDs suggests that the Stark peak in the Mn^{2+} doped QDs occurs due to development of an electric field in these QDs. The delayed appearance of electric field can be explained by the oxidation of Mn^{2+} by holes and the subsequent reduction of Mn^{3+} by electrons from the $1S_e$ state with the formation of excited $\text{Mn}^{2+}(\text{d}^5)^*$ ions. The revealed Stark peak suggests a charge-transfer mechanism of Mn^{2+} excitation by the band-edge exciton, it differs from the non-radiative energy transfer mechanism, which does not imply the development of an electric field in the QDs. The excited Mn can act as a reservoir of excitation energy, which promotes the generation of “hot” electrons involved in photocatalysis. The

talk discusses the problem of relaxation of “hot” excitons, generation of “hot” electrons, and their participation in the photocatalytic reduction of protons to molecular hydrogen.

Aknowledgments. This work was supported by Russian Science Foundation (grant number 17-13-01506).

T6-PL: Nano-scale fabrication of graphene based devices

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²*Faculty of Physics, University of Bucharest, Romania*

Graphene based devices represent a possible solution for the nanoelectronics of the future. Their functionality of strongly depends on the shape of the graphene itself. Unpatterned graphene has no bandgap, being not suitable for the fabrication of many devices as for example the digital field effect transistors, because the “off state” could not be achieved [1]. The very high resolution and great flexibility of electron beam lithography recommend this patterning technique as a very useful tool for shaping graphene and for fabrication of graphene based devices that feature very often details in the sub 100nm range. This presentation will be focused on nanoscale patterning of graphene for the fabrication of various devices: graphene diodes for high frequency applications [2], ballistic transistors producing negative differential resistance with large peak to valley ratio [3], back gated field effect transistors used as test devices to study the effect of for electron beam irradiation of graphene and graphene photodetectors with plasmonic structures [4], or graphene FETs with nanopatterned channel (fig.1). For all these devices the

graphene was patterned by electron beam lithography and etched by RIE in oxygen plasma, using as protective layer two electron resists: a positive one - PMMA and a negative one - HSQ.

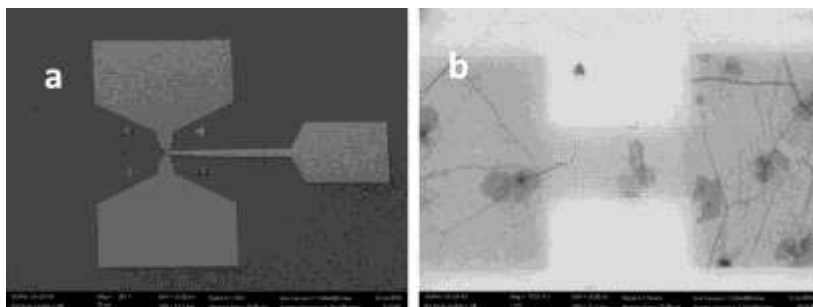


Fig. 1. Graphene based field effect transistor (a) and nanopatterned graphene channel (b)

The advantages and drawbacks presented by these resists are analyzed in relationship with the effect of electron beam irradiation of graphene, revealing important consequences for the fabrication and characterization of graphene devices and in particular for those steps in which e-beam lithography or scanning electron microscopy are involved.

- [1] A.K. Geim, K.S. Novoselov, Nat. Mater., 6 (2007), p. 183
- [2] M. Dragoman, A. Dinescu and D. Dragoman, European Solid-State Devices Research Conference, Bucharest, Romania, 16-20 September 2013
- [3] M. Dragoman, A. Dinescu, D. Dragoman, "Negative Differential resistance in graphene based ballistic field-effect transistor with oblique top gate nanotechnology" (vol 25, no 41)
- [4] A. Dinescu, M. Purica, R. Gavrilă, A. Avram, R. Müller "Influence of Low Energy Electron Beam Irradiation of Graphene Ribbon

Based Back Gated Field Effect Transistors", MRS 2012 spring meeting, April 9-13, San Francisco, California.

Plenary, Invited and Oral Sessions

HALL 1 – 15:00

T12-PL: NanoArt as Visual Aid in Nanoscience and Nanotechnology

Cristian Orfescu¹

¹NanoArt21, Los Angeles, USA

To ease the learning difficulties associated with various concepts that exist at microscopic scale, visual models are used more frequently. Complex micro and nanostructures cannot be visualized with naked eye and students have to develop a number of new skills to be able to observe matter at this level. Visual literacy in science and technology education is becoming a necessity due to the rapid integration of new technologies. This presentation is introducing NanoArt as a visual aid for education in Nanoscience and Nanotechnology in order to understand the benefits of the integration of this new artistic-scientific discipline in a future school curriculum. The evolution of the visibility power and visual theory which made all these developments possible and a short primer on electron microscopy are also presented. Finally, the events sponsored by NanoArt 21 organization in its 17 years of existence are mentioned.

T12-I: The Sound of Nano: The nanomaterial silica aerogel as a priceless piece of sky for high jewellery design

Ioannis Michlaoudis¹

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Today's high technologies for advanced materials tend to be developed and performed by a handful experts, and sometimes the principles and fundamentals of the technology are invisible by the general public. By contrast, at the same time, those knowledges can also offer attractive features on the society through design of materials/products, which can stimulate both sides for development in unprecedented ways. This paper summarizes the author's recent challenges on fusion between science and visual arts. Here, with the ethereal NASA's nanomaterial silica aerogel as an example, we demonstrate how the synergies between science and art has been developed and interactions between the material and artistic awareness stimulated each other through high-level mutual understandings. Silica aerogel makes itself a unique material by its beauty warranted via a high visible-light transparency and an unparallel porosity. Typically prepared through the sol-gel process from alkoxysilane precursor such as tetramethoxysilane (TMOS), silica colloids are developed by the hydrolysis and polycondensation, and they form thin solid skeletons by linking together three dimensionally. The resultant nanostructure and appearance of a typical silica aerogel creates a thinskeletons of ~10 nm for the mesoporous framework in the size range of ~50 nm, which minimizes the

Mie scattering and allows transparent appearance. Meanwhile, due to the Rayleigh scattering by the colloidal network, silica aerogel looks bluish, for the similar reason to the blue sky. The conceptual understanding of silica aerogel as the personification of heavens, induced the authors' idea of creating sky sculptures since 2002 in a man-made nanomaterial, which evoked applications of chemical and engineering technologies to visual arts and design. Particularly in this paper we underline an application of the nanomaterial silica aerogel on the design of high jewelry.



Fig. 1.a-c. Contemplation collection, July 2020, Skydrop pendant and bracelet, Courtesy of Maison Boucheron, Paris, France, EU.

Starting 2018 and for two years, Dr. Michalou(di)s had collaborated with Claire Choisne, the creative director of the jewelry company Boucheron for the creation of the first-ever silica aerogel high jewelry "Goutte de ciel", Skydrop, Fig.1.a-c. A deluge of Skydrops having a glass sound composing the nano soundscape of this presentation... We believe the present paper will enhance the needed communication between science and society where "inspiring" has to have an added value.

T12-I: How to draw an electron: Physics as a feature and method for art

George-Byron Davos¹

¹Athens News Agency - Macedonian Press Agency, Athens, Greece

A perennial concern for every artist has always been the question about how it might be possible to represent by means of the physical attributes of his/her craft the objective or inner reality of the natural (both human and physical) matters. Or, to paraphrase Austin's premise, how would it be possible to make things with artistic language. In fact, how is it possible for an observation, even if it is macro-empirically unnoticeable, to be representable?

Drawing on the well-known dispute about Drexler's insistence in seeing Nanotechnology as a pure mechanical system, discounting till the complete loss of the multiform and vital mutability and semantic variability of such a living matter like the nanomaterials are, the aforementioned works of Pollock and Vermeer's as a fine example of the hybridization of two interacting models of "Weltanschauung". Painting, finally is derived, is about matter and about its conditions and properties in the same way science works with it.

To advocate this argument, it is necessary to remind that there were times when the artist was considered also a scientist. Or, inversely, a scientist on many occasions resorted to an artistic-like paradigm, or model of representation of his theories, to vulgarize, or explain plainly in a parrot-like language the

achievements, the discoveries, and the modality of the function of the discipline principles of his field.

Similarly, to the scientist, who during a scientific experiment tries to determine the time and the space covered by a particle through the achieved trajectory, the painter looks for the definition of his/her artistic gesture by capturing the elementary traces and pictographical elements that constitute the entire body (and not just the surface and the represented features) of a picture, or more likely the act of painting as a whole. In Pollock's paintings all the overlapping trajectories of paint could be reasonably paragoned with the enactment of a scientific experiment, where the calculated initial goals and intentions, as well as the result of the whole endeavour, are dependent on the randomness of an electron's trajectory, or the paint's spilling.

Also, in this act is fulfilled a prominent requisition that states that in the space a shape, a figure, or an act, can be repeated, be superposed to another and never be exactly the same--as it supposed to be a brushstroke.

However, there lies the possibility and challenge at the same time of an interdisciplinary collaboration of the two different points of view. Whereas the artist explores the reality of the world by engaging different paths than those of science and incorporating the breakthroughs of the standing , "standard", theories produced by the scientific experimentation, the properties of the matter as they are understood through the prism of the creative mind and consciousness, give rise to a vision that in the bottom line does not differ much from the ideal form a scientific way of thinking has introduced as model.

T12-I: Symmetry Across Disciplines

Anna Ursyn¹

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Symmetry can be seen as a merger of various disciplines as most observe its presence recorded in different ways. Each professional understands it according to one's own discipline's code, so it might be interesting to see how this phenomenon differs across various fields of study and find matters of joint interest. This text offers several ways we can think about the vast theme of symmetry (and asymmetry) we encounter every day in our reality, reasoning, and aesthetic judgments. First, it examines some instances drawn from mathematics and sciences: geometry, physics, chemistry, computer graphics, and then biology, psychology, and medicine. Further text is focused on human culture, telling about symmetry in the arts, pattern design, aesthetics, and architecture. Finally, diversity of instances of asymmetry tells us how the absence of symmetry may modify form and functions of inanimate and living structures.

T12-I: Emergence of Natural Order

Samantha R. Lish¹

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How do intricately organized multi-cellular complex life forms emerge from the chaotic disordered activity of individual

particles? In nature, this phenomenon of self-assembly accompanies characteristic patterns of growth that appear in developing structures. However, the mechanism by which growth is coordinated on larger scales remains unknown, because disentangling non-linear dynamics in phase and shape space from aggregates remains a challenge. From the perspective of condensed matter theory, biology is an emergent collective phase of active soft particles that exists in a perpetual state of movement away from equilibrium. At the many-body particle level, non-equilibrium thermodynamic states arise due to dissipation of energy gradients, which plays a significant role in sustaining physiologic conditions that support life. Understanding the robust set of geometric conditions that involve cells moving as a collective rather than as single bodies can be modeled as a sum of probabilistic and fluctuating parts, which has broader implications about plasticity and morphogenesis. While typically relegated to describing the infinitesimal actions of particles that seem far away from relevant human application, advances in the field of mathematical and theoretical physics have demonstrated that there is crossover between the microscopic and macroscopic worlds. This transformation of an amalgam of abstract parts and geometries into meaningful information is the subject of my scientific and artistic endeavors to uncover universal laws and truths inherent to human creativity and natural wonder.

T12-I: Nano-Structure Surface Visualization in Mathematics, Applied Sciences, and Art

Jean Constant

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The exploration of minimal surfaces is a field of research that permeates many disciplines, from mathematics, applied sciences, biological and physical sciences, even architecture and art.

Surfaces that locally minimize area have been utilized extensively to model physical phenomena such as soap films, black holes, compound polymers, protein folding, etc. As a result of their anticipated and consequential outcomes, many researchers investigate this field, particularly in molecular engineering, materials science, and nanotechnology [1].

The Schwarz family of surfaces is self-contained and expendable from nano level to infinity. Its symmetry component creates an appearance of stability and harmony. Data visualization [2] is a fundamental skill in data science. It can be used as a separate means to explore, understand, and communicate results. The author explored the initial Schwarz surface structure using the framework of Knowledge visualization [3] that proposes a path that bridges the comprehending gap between art and science and adds to the larger discourse relating to the understanding and communicating of a visual statement.

Accordingly, the author investigated the shape of the surface in a modeling program and combined the results in a graphics editor to add elements of color and density to a flat 2d visualization that could be understood and appreciated both by a researcher and a general audience.



Fig. 1. 3D model rendering of a Schwarz surface

His experiment led him to conclude that visual communication techniques [4] are significant tools in sharing information. Additionally, they help initiate a dialog in which the viewer's imagination may lead them to investigate further information of a scientific nature, awaken additional curiosity in scientific research, and boost interest in science education and future careers in the scientific field.

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T12-I: Explorations of the Invisible Domain: Art and Science meet at the Hopkins Extreme Materials Institute

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² *Art Academy University, San Francisco*

The Extreme Arts Program at the Hopkins Extreme Materials Institute is a collaboration between Johns Hopkins University (HEMI) and the Maryland Institute College of Art (MICA) in Baltimore, Maryland. The program, funded by the National Endowment for the Arts, provides a unique opportunity for art faculty at MICA to interact with researchers at HEMI.



Fig.1. One of the pieces created in the 2019 Extreme Arts Program at the Hopkins Extreme Materials Institute.

As the 2019 artist-in residence for this program, I was able to collaborate with three HEMI researchers and their labs to create art inspired by their work.

The artwork included 3D printed models and large prints. My particular interest was to explore new ways to visualize things that are beyond human unaided vision, such as atoms and molecules (Fig.1). This presentation will include a discussion of some of the strengths and weaknesses of artist-scientist collaborations like this.

It will also include a discussion of the process involved with the creation of art for this project.

Poster Session I

HALL 1 – 18:05

T1-P: Studies on the structure, optical and electrical properties of $\text{In}_{2-(x+y)}\text{Sn}_x\text{Zn}_y\text{O}_{3-\delta}$ thin films deposited by spin-coating

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Thin films in the system In-Sn-Zn-O were deposited on different substrates (glass, quartz, nSi, pSi) by spin coating. The content of Sn+Zn was maintained constant, 20%, selecting two situations: 14% Sn; 6% Zn and 6%Sn, 14% Zn, by mixing certain solutions of zinc acetate, indium chloride and stannous chloride in DMF. The influence of co-doping on the structure, optical and electrical properties was investigated. The thin films show a cubic byxbeite structure and a transmittance higher than 80%. Current voltage curves and Hall measurements enabled to have information about the p-type or the n-type character of thin films, for high Zn content or high Sn content respectively.

T1-P: Structural and electrical investigations on a junctionless transistor with a Si co-doped channel

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³*Faculty of Physics, Alexandru Ioan Cuza University, Iasi, Romania*

Working junction-less transistor become possible due to SOI technology. Junction-less transistors require high doping ($>10^{19}$ atoms cm^{-3}) to ensure a high current drive and to minimize contact resistance. We performed I-V measurements, for junctionless transistors with uniform high co-doped Si channel and we were interested in the influence of channel size effect on transport mechanism. Some measurements performed at low temperature seemed to be close to the results obtained in the literature for the highly doped Si with P. For $V_g=0$, the Coulomb gap and the resistance anomaly was observed. A decrease in maximum resistance value and an increase of resistance peak width with increase in the the channel width was observed. At room temperature the zero anomaly disappears, and current-voltage characteristics become resistive.

T2-P: Angle- and time-resolved in situ investigation of pulsed laser deposition of Cu_xO_y semiconductors

S. Irimiciuc^{1,2}, S. Chertopalov², M. Novotný², M. Vondracek², J. Lancok², V. Craciun^{1,3}

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A wide range of plasma diagnostic tools based on Langmuir Probe (LP) and Optical Emission Spectroscopy (OES) were used to investigate the pulsed laser deposition of p-type semiconductors based on copper oxides. Different routes for thin film formation were investigated starting from either Cu or CuO in O₂ atmosphere. Plasmas generated from a CuO target were defined by a higher plasma potential and electron temperature as observed by time-resolved LP analysis, which affected the kinetic energy of the particle during expansion. The effect of gas addition (O₂) on the copper oxide plasma dynamics was also investigated. Angle resolved measurements revealed a complex distribution of the ions with positive species ejection at large expansion Angles in CuO plasma, attributed to oxygen species presence as they were not observed in the Cu target ablation in O₂ case. Plasma potential, charge density and electron excitation temperature were increasing with the gas pressure while electron temperature and expansion velocities were decreasing. Using a semi-empirical model, estimation of ion acceleration field, neutral temperature and densities were performed. Space- and time-resolved OES confirmed the plume splitting indicated by LP measurements and provided insight into the plasma multiple structuring scenario. All the plasma parameters were investigated in conditions similar to those used for thin films growth and the results are discussed with respect to the pulsed laser deposition (PLD) technology.

Comparison between the properties of the plasma and those of the deposited films are made.

T2-P: Analysis of laser produced plasma on various metals: ion current interpretation by floating probe approach

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³*Laser, Extreme Light Infrastructure for Nuclear Physics, Magurele, Romania*

Complementary optical and electrical diagnostic tools were implemented for analysis of transient plasmas generated by ns-laser ablation of Cu, Bi, Ag and Co. The dynamics of the transient plasmas were investigated in different scenarios by introducing both inert and reactive gases. The focus of our work was on implementing the floating Langmuir probe regime for plasma analysis and the time-of-flight semi-empirical models to completely characterize the kinetic and thermal energy of the plasma used in pulsed laser deposition (PLD). In depth angular measurements were aimed at understanding the plasma plume distribution during PLD process and how structural defects and deviation from stoichiometry can be related to the plume heterogeneity. Multi-peak structures were seen for all metallic plasmas with a good correlation between the atomic mass and melting point of the target and the charge density and ion kinetic energies. This feature was observed due to different arrival time of single and multiple ionized species (Cu, Bi, Ag, Co), aspect confirmed by optical time of flight investigations, where the space-time separation was also seen. The energetic structuring of the plasma also appeared in the context of time-resolved I-V characteristic for

short evolution ($< 1 \mu\text{s}$) times, where strong wave-like behavior was noted. The origin of charged particle oscillation was analyzed in the framework of highly ionized fast expanding plasmas and what could be its measurable impact on the pulsed laser deposition process. Finally, the nature of the saturation current measurements in fast expanding plasmas is discussed and confronted with these new results.

T3-P: Environmental friendly laboratory method for PGM recovery from spent auto converters

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Platinum Group Metals (PGMs), which includes Platinum (Pt), Palladium (Pd), Rhodium (Rh), Osmium (Os), Iridium (Ir) and Ruthenium (Ru) are widely used in various applications due to their excellent proprieties such as: thermoelectric stability, corrosion resistance, high electrical conductivity, catalytic activity. Therefore, many industries depend on PGMs sustainability and availability. The automotive industry is one of many industrial applications of the PGMs as catalytic converters (Three-Way-Catalyst (TWC) or Diesel-Oxidation Catalyst (DOC). The primary PGMs sources are strongly geographically limited, which makes the spent automotive catalysts the biggest secondary PGM resource. As, there is growing demand for the metals and also considering the negative impact of these spent catalyst on the environment, the recycling of PGMs from automotive catalysts is indispensable. The recovery of PGMs

from the spent catalyst can be complex due to the presence of different components in the catalytic support and also to the alteration of initial catalyst structure during many hours of usage. The objective of this study was to establish an efficient and eco-friendly laboratory method for recovering the PGM from the spent auto catalysts by employing different experimental conditions. The studied samples came from a spent automotive catalyst that had become deactivated under real traffic conditions. The powder used further for characterization and Pt, Pd and Rh recovery was obtained by crushing the catalysts in a planetary ball mill. The spent automotive catalyst samples were characterized using different characterization techniques such as: XRD, XPS, TGA. The PGMs recovery was achieved in two steps: (i) metal solving in $\text{H}_2\text{O}_2 + \text{HCl}$ solution and (ii) metal recovery from solution. For a high degree of recovery in the dissolving step we have varied different parameters like: leaching agent concentration, the temperature and the extraction time. Furthermore, different precipitation techniques were employed in order to separate the individual ions from the leaching solution and to obtain high yield and purity for recovered PGMs.

T3-P: Electrochromic prototype devices based on triphenylamine-triphenylmethane containing polyimides

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Electrochromic materials that exhibit a reversible optical change upon electrochemically oxidation or reduction can be grouped in transition-metal oxides, inorganic coordination complexes, conjugated polymers, and organic molecules [1]. Although the electrochromic devices are mostly based on inorganic oxides, the organic materials have several advantages, such as processability, high coloration efficiency, fast switching ability, and multiple colors within the same material. Generally, the investigation of electrochromic materials has been directed toward optical changes in the visible region (e.g. 400–800 nm), which proved to be useful in various applications, such as E-paper, optical switching devices, smart window, and camouflage materials [2]. Among electrochromic active structures, triphenylamine (TPA) is one of the most studied moieties since it is easily oxidized to form stable radical cations, associated with a strong color change. On the other hand, polyimides are rank among the most heat-resistant polymers and are widely used in high temperature applications, including the fields of aerospace, defense, and opto-electronics; they are also used in liquid crystal alignments, composites, electroluminescent devices, electrochromic (EC) materials, polymer electrolyte fuel cells, polymer memories, fiber optics, etc. [3]. In this context, a novel structural strategy towards triphenylamine (TPA)-modified polyimides has been approached by starting from a TPA-functionalized triphenylmethane (TPM)-based diamine with electrochromic response. Based on these polyimides, EC prototype devices were ansambled and the main parameters were evaluated.

Acknowledgements: This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, Project PN-III-P2-2.1-PED-2019-3520, 438PED/2020, within PNCDI III.

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T3-P: The recycling of spent plates from car batteries and the doping with cobalt (II, III) oxide

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The recycling methods currently applied in the field of the spent plates from lead-acid batteries are those of pyrometallurgy and hydrometallurgy. These methods have some major drawbacks including: high efforts to convert back to metal oxide, inefficient desulfatization, complexity and toxicity for the atmosphere [1]. Due to these shortcomings, the melt-quenching method inspires the recycle and the reuse of spent electrodes of the car battery [2]. The second problem regarding electrodes implies the decreasing the life of car battery. The main inconveniences that yield to the rapid discharge of the car battery are the phenomena of anodic passivation and the evolution reactions of hydrogen. In this study, new vitreous systems in the $x\text{Co}_3\text{O}_4 \cdot (100-x)[4\text{PbO}_2 \cdot \text{Pb}]$ composition where $x = 0 - 25$ mol% Co_3O_4 were prepared by melt-quenching method using as raw

materials the spent plates (the anode as Pb source and the cathod as PbO₂ source, respectively) of a car battery. The structural and electrochemical properties of the samples were investigated by X-ray Diffraction (XRD), InfraRed (IR) and Electron Paramagnetic Resonance (EPR) spectroscopy, measurements of cyclic voltammetry (Fig.1).

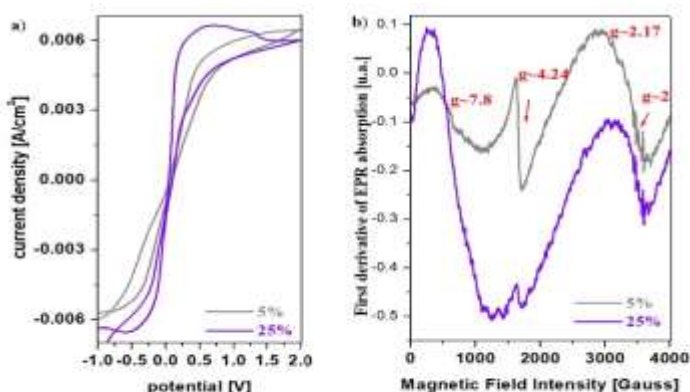


Fig.1. a) Cyclic voltammograms and b) EPR spectra of the recycled and cobalt-doped materials in the $x\text{Co}_3\text{O}_4 \cdot (100-x)[4\text{PbO}_2 \cdot \text{Pb}]$ composition where $x = 5$ and 25 mol% Co_3O_4 .

Analysis of the X-ray diffractograms indicates an abruptly decrease in the sulfatized phases content and an increase of lead oxides phase amounts by the addition of higher Co_3O_4 contents. By doping the IR data show: i) a decreasing trend in the intensity of the bands assigned to sulfate ions and ii) a conversion of $[\text{PbO}_3]$ pyramidal units into $[\text{PbO}_4]$ tetrahedral units. EPR spectra evidence the resonance signals centered at about $g \sim 2$, 2.17, 4.24 and 7.8 corresponding to the Co^{+2} ions with octahedral and tetrahedral sites. Measurements of cyclic voltammetry suggest that the recycled and doped electrode

materials with a higher content of cobalt double oxide can be reused as new energy sources in lead-acid batteries.

Acknowledgements: This paper was supported by the Ro-Dubna projects, Protocol No. 56 / 2021.

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T3-P: Enhanced visible light activated mesoporous titania by rare earth metal doping

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Nowadays, one of the major challenge of humanity is the improvement of water and air quality. It is well known that when metal oxide semiconductor nanoparticles, such as TiO₂, are used as photocatalysts, the major challenge is to obtain a photoresponse in the visible range. During this study, this was achieved by doping titania with rare earth metals (Ce³⁺, Dy³⁺, La³⁺, Sm³⁺). The doped mesoporous titania was synthesised by an ultrasound-assisted method, using Pluronic F127 as pore structuring agent. Microwave technique was involved in order to achieve surfactant removal. The properties of the synthesized samples were investigated by N₂ sorption/desorption technique, X-Ray analysis, TEM imaging and Diffuse Reflectance UV-vis Spectroscopy.

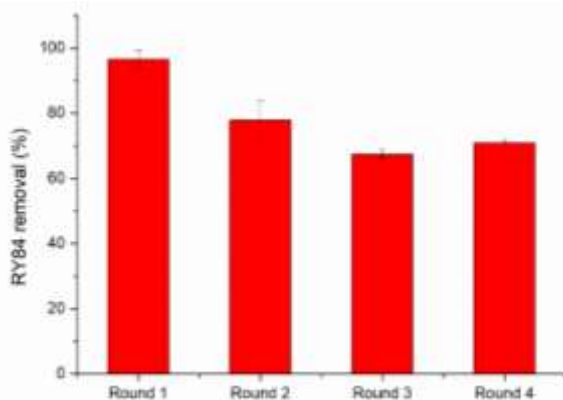


Fig.1. Adsorption and photocatalytic removal of RY84 by Sm-TiO₂ sample over 4 consecutive cycles

The new synthesised materials provided increased specific surface area, improved bandgap energy values, promoting a photo-response in the visible range. The efficiency of these materials was studied for the visible light photodegradation of Reactive Yellow 84 dye, with very good results: 96% dye removal in the case of Sm-TiO₂, after 140 min reaction time. 70% dye removal was achieved after 4 cycles of reuse in the case of the same powder. These findings are explained by the advantage of the doped materials to ensure the transport of the charge carriers and to avoid the recombination of the photoinduced electron-hole pairs, thus maximizing the photocatalytic process.

In our work, coconut shell has been selected as biomass precursors to obtain AC and then applied as electrodes for SC and electrode for PSC. As a result, ACs are readily produced from coconut shell waste using eco-friendly activation processes with water and steam treatment. The storage

properties of activated carbon electrodes were found to be in close relationship with the morphological and structural properties of the precursor material. Among the samples prepared, the AC showing high surface area ($1998 \text{ m}^2\text{g}^{-1}$) in contact with ionic liquid (MPPyFSI) displayed outstanding SC storage capability.

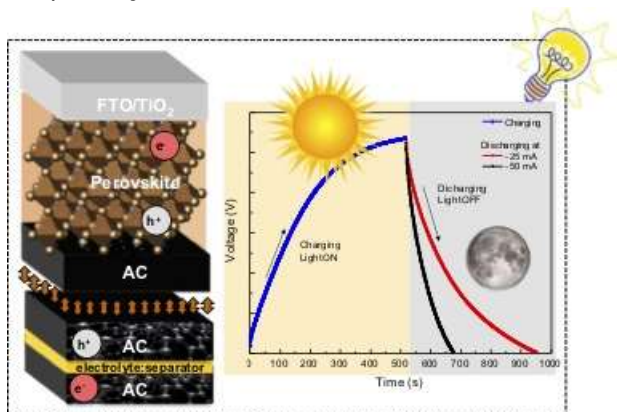


Figure 1. Integrated device: carbon-PSC/carbon-SC.

The capacitance of 219.4 F g^{-1} with a specific energy of 92.1 Wh kg^{-1} and power density of 2046 W kg^{-1} at 1 A g^{-1} were obtained with retention of high values at a current density of 30 A g^{-1} .² Preliminary results of the integrated system: carbon-PSCs/carbon-SCs were obtained and will be discussed.

Acknowledgements: Programme d'Investissements d'Avenir, ANR-19- MPGA-0006.

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T3-P: Thermal characterization of MOFs in the cryogenic temperature domain by photothermal techniques

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Green hydrogen is considered as an energy vector to reduce greenhouse gas emissions and pollution. Its deployment requires reservoirs that can be made up of nano-porous organometallic structures such as MOFs (Metal-organic frameworks). Their adsorption/desorption efficiency phases depends on the storage capacities of the MOFs but also on their thermal properties. MOFs are a unique class of crystalline materials with very high porosity (up to 90% by volume) and a gigantic specific surface area (up to $6000 \text{ m}^2 \cdot \text{g}^{-1}$). It is necessary to intensify research on storage capacity of MOFs in order to obtain an operational reservoir. Promising materials with an appropriate balance between porosity, pore size distribution and compaction density are extensively studied. The thermal properties of materials for hydrogen storage directly influence the performance and efficiency of physisorption-based systems. The utility of MOFs for gas storage depends on their ability to rapidly dissipate heat generated during the exothermic adsorption process. The thermal conductivity of the adsorption substrate controls the rate of H_2 adsorption/desorption. Low thermal conductivity creates

thermal gradients which can prevent the adsorption of hydrogen. A high thermal conductivity is thus necessary to remove heat from the network very fast, in order to establish the optimal operating conditions. It has recently been shown that an increase in thermal conductivity by adding graphene as additive tincreases adsorption/desorption kinetics by a factor of 4 compared to MOFs without additions [1]. The equilibrium time required to reach 90% of the maximum hydrogen adsorption capacity is reduced by 25% for pellets with an improved conductivity [2]. Understanding the principles of thermal transport in MOFs is critical to enable these materials to reach their full potential for H₂ storage. There are few studies on improving the thermal conductivity of MOFs, particularly at cryogenic temperatures. PPE calorimetry at room temperature with a contact fluid, photothermal radiometry (PTR) and lock-in thermography (LiT) have been used for thermal characterization of MOFs [1,2]. The objective of this study is to determine, without coupling fluid and at atmospheric pressure, the thermal effusivity of MOFs from -180°C to ambient by PPE calorimetry technique. It is possible to determine the effusivity of MOFs without altering their porosity and thus to deduce their thermal conductivity within the cryogenic temperature range for which they are intended.

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T4-P: Magnetic properties and magnetocaloric effect in La_{0.7-x}EuxBa_{0.3}MnO₃ compounds.

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Structural, magnetic properties and magnetocaloric effect of La_{0.7-x}Eux Ba_{0.3}MnO₃ bulk material with $x = 0, 0.05, 0.1, 0.2, 0.3$ and 0.4 have been investigated. The compounds were prepared by solid-state reaction method. The structural properties were investigated by powder X-ray diffraction. Lattice parameters obtained from XRD measurements tend to slowly diminish with increasing Europium content. Morphological properties were studied using a Scanning Electron Microscopy and show an increase of grain sizes with increasing doping level was seen. Oxygen stoichiometry was determined by Iodometry which indicated that the compounds have a slight oxygen deficiency. Magnetic measurements were done using Vibrating Sample Magnetometer in the range 4-300K. The analyzed samples display ferromagnetic order below TC and systematic decrease in TC caused by doping. For Europium level of $x = 0.05$ the sample displayed a room temperature TC. Magnetic entropy change was determined from magnetic isotherm measurements for 0.05, 0.1 and 0.2 compound. A large magnetic entropy change and a high

relative cooling power were found, which are promising for application in magnetic refrigeration

T4-P: STRUCTURAL AND MAGNETIC PROPERTIES OF Gd Co_{2-x} Ti_x COMPOUNDS

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Structural and magnetic properties of the intermetallic GdCo_{2-x}Ti_x (x=0.05, 0.1, 0.2, 0.3, 0.4) compound were investigated. The materials were synthesized by arc melting, followed by a thermal treatment at 900°C. The structure was analyzed using X-ray diffraction. Magnetic measurements were performed with a VSM in magnetic fields up to 12 T and temperatures between 4-300 K and with a Weiss type scale in the 300-500K temperature range. The compounds crystallize in cubic Laves phase. The samples with x=0.05 and 0.1 are single phase. Small amount of Gd₄Co₃ was detected for higher Ti concentrations. The lattice constant is not changing with doping being around 7.26 Å, fact explained by the very small differences between the ionic radius of Co and Ti. All the samples are ferrimagnetically ordered, with the Gd and Co(Ti) magnetic moments antiparallely oriented. The Curie temperature varies little with composition and remains in the range T_c=394-399K, close to 404 K, the GdCo₂ transition temperature. Finally, the influence of titanium atoms substitution on cobalt site is discussed.

T4-P: Electronic structure and magnetic properties of $\text{GdCo}_{2-x}\text{Mn}_x$ Intermetallic Compounds

51

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²*Physics, University of Osnabrück, Osnabrück, Germany*

The electronic structure and magnetic properties of $\text{GdCo}_{2-x}\text{Mn}_x$ compounds with $x = 0.1, 0.2$ and 0.3 have been investigated by XPS and magnetic measurements. The powder X-ray diffraction measurements show that all samples are single phase and crystallize in the cubic MgCu_2 (C15) structure. The lattice parameter was found to increase slowly with the manganese content. The magnetic measurements were performed in magnetic fields up to 12 T in the temperature range 4 – 800 K. All the investigated samples are ferrimagnetically ordered Gd and Mn magnetic moments being antiparallely oriented. Saturation magnetization determined at 4 K is decreasing with increasing manganese concentration from $4.89 \mu_B/\text{f.u.}$, for $x=0.1$ to $4.22 \mu_B/\text{f.u.}$, for $x=0.3$, while Curie temperature is increasing with manganese content from 438 K, for $x=0.1$ to 480 K, for $x=0.3$. Our analyzes show an increase of cobalt magnetic moment with the manganese content. Finally, the results obtained by XPS measurements are correlated with those obtained by magnetic measurements.

T4-P: Structural, Microstructural and Magnetic properties of $\text{SmCo}_5+20\text{wt}\%\text{Fe}$ Magnetic Nanocomposites Produces by Mechanical Milling in the presence of CaO

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High performance permanent magnets (HPPM), due to their large energy density (up to 500 kJ/m^3), are vital for a large variety of applications, from mobile phones and computers to wind turbines and electric vehicles. However these materials can currently only be obtained using rare earth elements (Nd, Sm, Dy etc). This is a significant problem as rare earth elements are obtained and processed only in certain regions of the globe, a fact which has lead to significant price fluctuations and scarcity in recent years. Moreover the extraction and processing of these elements comes at a significant environmental cost. Exchange coupled nanocomposite, a nanostructured magnetic material in which the high magnetization of a soft magnetic phase is stiffened by the high anisotropy of a hard magnetic phase, hold great promise for the future of permanent magnets, with a predicted energy density of up to 1 MJ/m^3 . However, due to the precise nanostructure control required, the synthesis of these materials has proven difficult. In this work, we show the possibility of using a soluble ceramic material, $5\text{wt}\%\text{CaO}$, as an additive for $\text{SmCo}_5+20\text{wt}\%\text{Fe}$ exchange coupled

nanocomposite in order to inhibit the grain growth of the hard and soft magnetic phases. Magnetic measurements show that the presence of 5 wt% of CaO during nanocomposite processing significantly improves the coercivity of the SmCo_5/Fe nanocomposites by inhibiting the grain growth of the soft magnetic phase.

We acknowledge the financial support from the UEFISCDI, Romanian Ministry of Research, Innovation and Digitization, grant PN-III-P2-2.1-PED-2019-4696.

T4-P: The $(\text{Co-Fe})_f$ ferrite biocompatible magnetic nanoparticles for increasing efficacy and reducing toxicity in superparamagnetic hyperthermia for alternative cancer therapy

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In alternative therapy of cancer by magnetic hyperthermia the most important issues for increasing the effectiveness of the method are finding the most suitable biocompatible magnetic nanoparticles and the optimal conditions for alternating magnetic field [1–4]. In this paper we propose an innovative nanobiomaterial based on magnetic nanoparticles of $(\text{Co}_x\text{-Fe}_{1-x})\text{Fe}_2\text{O}_4$ ($x=0\text{--}1$), denoted $(\text{Fe-Co})_f$, biocompatibilized with polyacrylic acid (PAA-500, Sigma Aldrich,) for its use in

superparamagnetic hyperthermia (SPMHT) of cancer with high efficacy and lack of toxicity. The biocompatible magnetic nanoparticles were characterized by XRD, FTIR, XRF, DLS techniques and magnetic measurements. Our 3D computational study shows that the optimal size of ferrimagnetic nanoparticles for obtaining the maximum specific loss power (Ps) and quick heating of magnetic nanoparticles at temperatures of 42–43 °C required in magnetic hyperthermia to destroy tumor cells, strongly depends on the concentration of Co^{2+} ions in $(\text{Fe-Co})_f$ ferrite structure for $x = 0$; 0.05; 0.1; 0.2; 1, and the thickness of the organic layer on the surface of nanoparticles (Fig. 1).

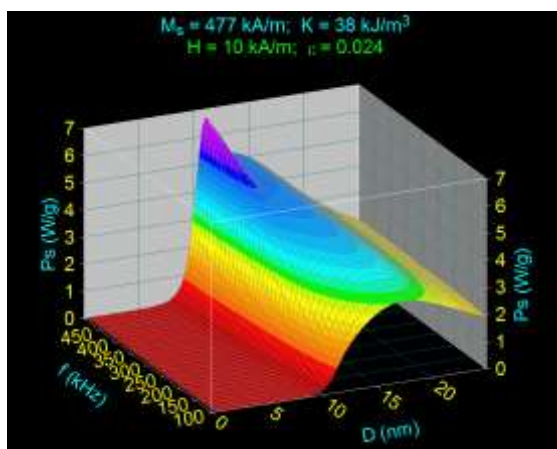


Fig. 1. The 3D variation of the specific loss power as a function of the frequency of magnetic field and the diameter of biocompatible $(\text{Fe-Co})_f$ nanoparticles for $x = 0.05$.

Thus, in the optimal conditions determined by us for obtaining SPMHT with maximum efficacy in the admissible biological limit

[5], we found that the optimal diameter (D_o) of magnetic nanoparticles must be in the range ~11–16 nm, the amplitude of magnetic field (H) in the range of 10–30 kA/m, and the frequency (f) in the range of 500–167 kHz. The use of SPMHT under the conditions established by us leads to major benefits in the implementation of SPMHT for cancer therapy *in vivo* and future clinical trials.

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T6-P: Thin layer gold-based substrate for pathogens SERS detection and quorum sensing monitoring

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This work focuses on the use of metallic thin layer-based substrates towards application in surface enhanced Raman scattering (SERS) sensing, in particular for ‘real-life’ applications.

We used a simple, single-step and effective method to create a gold thin layer-based SERS-active substrate for pathogens' detection and quorum sensing monitoring. A multi-assay capacity is also provided by ten microchannels carved from double-faced tape and fixed between glass slides.

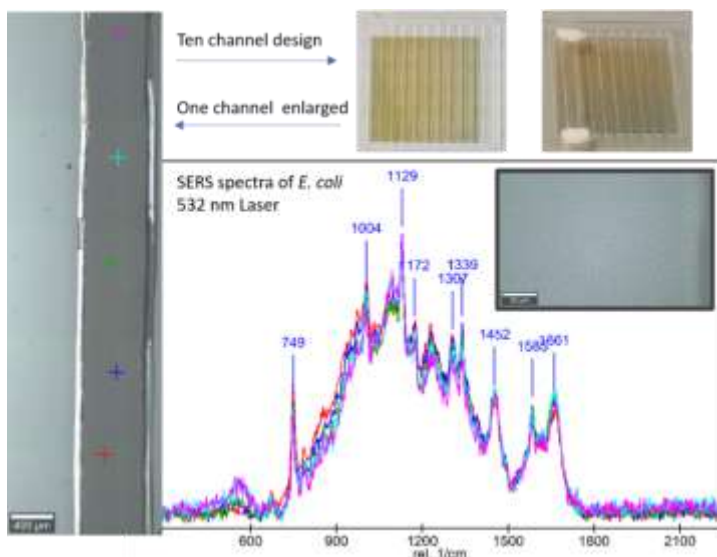


Fig. 1. The thin layer gold-based miniaturized SERS-active substrate showing all ten microchannels that can be used for multi-assay detection. One channel is enlarged for a better visualization and *E. coli* SERS spectra are shown, including the peak values for the main SERS bands.

The glass cover on top was firstly sputtered with gold by using a DC sputtering technique with two major advantages: it is easy to control and is a low-cost option. The thin film deposited on glass kept the transparency of the glass and made possible sample visualization and laser irradiation through glass.

Thus, we herein report on the fast bacteria detection directly from a 3 μ L droplet of sample. The thickness of the Au layer was found to play a significant role in the SERS enhancement. Ready-to-use, simple, cheap and ultra-sensitive detection are the key aspects of our miniaturized SERS-active substrate. Acknowledgements: This work was supported by a grant of the Romanian the Ministry of Research, Innovation and Digitization, CNCS – UEFISCDI, project number PN-III-P1-1.1-PD-2016-0475, within PNCDI III.

Poster Session I 18:05 – 20:00

Online

T9-P: Investigation of nanoparticle-based platforms toward imaging and plasmonic chemo-photothermal therapeutics

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Despite the recent progress in cancer diagnosis and therapy [1,2], it remains one of the leading causes of death worldwide. Therefore, there is still a growing interest in the development of theranostic systems using nanotechnology.

These are based mainly on colloidal nanoparticles (NPs) that can be successfully used not only as agents for transport and

controlled release of drugs but also as contrast agents for diagnosis by imaging of tumors.

In this study, we aim to achieve a new hybrid material that combines chemotherapy with local hyperthermia in the NIR region based on plasmonic NPs. Our theranostic system is based on several key components: i) a component for diagnosis through non-invasive imaging -NPs ii) an intrinsic therapeutic component based on the ability of NPs to convert the absorbed energy into heat under NIR light excitation (photothermal component) and an extrinsic therapeutic component (chemotherapeutic component); iii) a multifunctional polymer coating to ensure stability and biocompatibility of nanoparticles and loading of the drug. We investigate two different shaped AuNPs: nanospheres (AuNSs) and triangular nanoplates (AuNTs). Both of them are synthesized using gelatin biopolymer as a reducing and stabilizing agent. For the chemotherapeutic component of the systems, NPs are loaded with the drug Doxorubicin through a pH-sensitive hydrazone bond.

By employing steady-state fluorescence, Fluorescence Lifetime Imaging Microscopy under two-photon excitation (TPE-FLIM), Raman spectroscopy, and a thermal IR camera, we compare the obtained systems. Finally, we prove that the AuNTs@gelatin-hyd-DOX system is more suitable to be used as a theranostic agent. The system was validated inside biological phantoms that mimic the cancer tumor environment.

Based on these results, we proved that the proposed theranostic agent is able to synergistically incorporate multiple functionalities for performing diagnosis, targeted drug delivery,

and imaging, resulting in a more effective and personalized medical treatment.

Acknowledgements: This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P1-1.1-PD-2019-0235, within PNCDI III.

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T9-P. PVP modified graphene oxide nanoflakes as contrast agents inside tissue-mimicking phantoms via two-photon-excited fluorescence lifetime imaging and confocal Raman microscopy

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Significant research efforts are currently invested into the improvement of therapeutic outcomes in cancer surgery by designing new contrast agents that enable a sensitive, real-time intraoperative guidance with a clear and deep difference between healthy tissue and tumoral lesions [1]. Owing to their special optical properties such as fingerprint Raman bands and intrinsic visible and near-infrared (NIR) fluorescence emission, graphene oxide (GO) nanoflakes appear as promising contrast agents for Raman and fluorescence

imaging of cancer tissues [2,3]. However, the clinical use of GO as fluorescent probes is limited due to their negligible emission at neutral pH. Herein, we modulate the photoluminescence of GO in both, acidic and neutral medium by coating them with polyvinylpyrrolidone (PVP), an amphiphilic, biocompatible polymer. The formation and stability of PVP-GO are analyzed by UV-vis-NIR spectroscopy, Raman spectroscopy, dynamic light scattering (DLS), and zeta-potential measurements. The fluorescence emission properties of PVP-GO at pH values relevant for biomedical applications are investigated via steady-state fluorescence measurements using multiple excitation wavelengths, from visible to NIR. The potential of the fabricated PVP-GO to operate as both, visible and NIR activatable contrast agents for cancer diagnosis is validated inside tissue-mimicking agarose-phantoms via two noninvasive techniques: scanning confocal Raman microscopy (CRM) and two-photon-excited fluorescence lifetime imaging microscopy (TPE-FLIM). The results show that the fingerprint Raman bands and intrinsic photoluminescent properties of PVP-GO nanoflakes enable their tracking inside biological phantoms by CRM and TPE-FLIM without the need for any additional label. We anticipate that this class of contrast agents is promising for applications in image-guided cancer surgery. Acknowledgements. This work was supported by a grant of Ministry of Research and Innovation, CNCS-UEFISCDI, project number PN-III-P4-ID-PCCF-2016-0142, within PNCDI III.

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T9-P: Carbon-dots functionalized silicon nanowires for enhanced viral sequence detection in microarray format

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¹Nanobiotechnology, IMT Bucharest, Voluntari, Romania

The detection of viral DNA sequences on microarray format depends on obtaining a good fluorescent signal coming from the labeled single-stranded DNA. In order to obtain an enhanced fluorescence, we explored the use of carbon dots modified with poly(diallyldimethylammonium – PDDA (CDs-A) and poly(ethyleneimine) – PEI (CDs-B) on a nanostructured surface comprised of photoluminescent silicon nanowires.

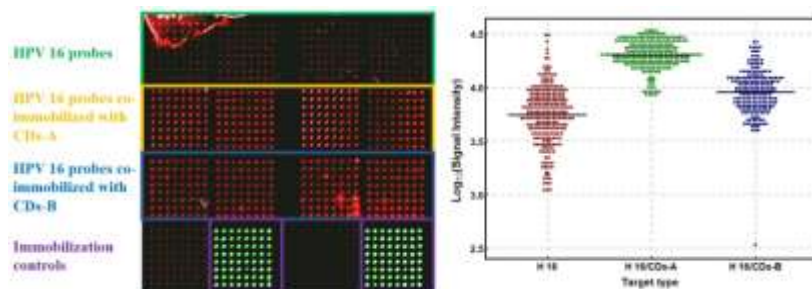


Image and graphical hybridization results on SiNWs platform.

The HPV 16 probes co-immobilized with CDs-A have shown best fluorescent enhancement.

This research presents the microarray results obtained on ssDNA fragments corresponding to HPV16, which were labelled with Cy5 by asymmetric PCR.

T9-P: Keratin-based polymer nanofilm membranes for medical applications

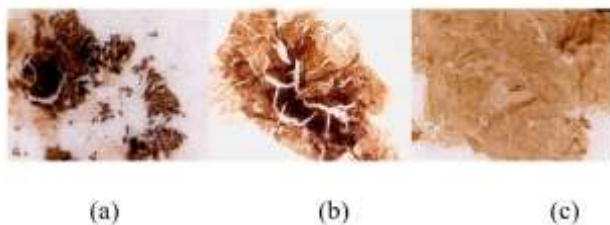
A. Cocean¹, I. Cocean¹, G. Cocean², C. Postolachi¹, B. Munteanu¹,
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¹*Faculty of Physics, Alexandru Ioan Cuza University of Iasi, Iasi, Roania*

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The experiments in this paper are part of a larger study, namely to capitalize on biomaterials available in nature for further medical applications. In this regard, a first step was to develop the method of obtaining thin layers of alpha-keratin using the PLD (pulsed laser deposition) technique using as a target composite biomaterials, namely horn and wool, and the results were published in 2019 [1]. The authors indicated at that time the planned medical applications, namely for transdermal patches and keratin membranes. The latter application, keratin membranes, is the subject of this work. The main issue that had to be addressed in a first stage is to obtain a polymer with continuous film properties and which can be easily detached from the surface on which the deposition by PLD was made. Physico-chemical treatments of alpha-keratin thin layer obtained by laser deposition on various substrates were performed.



Optical microscopy images of different experimental results after detaching the film for membrane from the substrate on which was produced

Through the obtained results, at least one of the methods used was identified as being efficient in obtaining a continuous film that could be easily detached by immersion in water at a temperature of 180 C. The chemical structure was investigated by FTIR Spectroscopy and optical microscopy (Figure 1), as well as electron microscopy revealed aspects related to the morphology and topography of the obtained films. Such a membrane could solve the problem of avoiding wound infection by a "temporary keratin graft" which can also act as a transdermal patch. Acknowledgments. This research was funded by Ministry of Research, Innovation and Digitization, project FAIR_09/24.11.2020

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T9-P: SEM imaging of nanomaterials adherent to the cell membrane

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Preparing biological specimens for scanning electron microscopy (SEM) usually entails critical point drying (CPD) processing of the samples. CPD, as a drying method, is not only expensive, but needs to be carefully implemented using specific parameters since small deviations can lead to damage of the sample [1]. On the other hand, drying the specimen directly in vacuum can incur other disadvantages such as cell deflation with consequent loss of specific morphology. In our case, the deflation was not a key parameter since the adherent nanomaterial was observed on the cell membrane. In this paper, we present the results obtained for samples which have been dried in the biological safety hood followed by vacuum. We tested the method using human osteosarcoma cells (HOS). Aim was to observe if Co-Fe nanowires (NW) (diameter 200nm, length 2 μm) were present on the cell surface after 24h of incubation with the cell sample. In parallel, we prepared a control sample in the absence of nanomaterials in the cell media. The cells were grown and fixed directly on sterilized silicon wafers.



SEM images of A. HOS B. HOS with NW adherent to the membrane

The fixatives include glutaraldehyde solution the presence of NW to the cell surface, as seen in the right image (B). We describe a novel cost efficient and easy to perform method for processing biological samples for SEM imaging that preserves cell morphology and can be used for describing nanoparticle interaction with cell surface. Acknowledgements - Work supported by (UEFISCDI) Contract no. PCE20/2021 (PN-III-P4-ID-PCE-2020-2381).

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T10-P: Fe-Cr-Nb-B glassy powders obtained by high-energy ball milling of amorphous alloy ribbons

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Amorphous and nanostructured magnetic materials (ribbons, wires, powders) have received great attention during the last decades due to their novel magnetic properties and potential

applications in high performance electronic devices, healthcare, and magnetic recording technology [1-3]. In this context, it is extremely important to understand how their reduced dimensionality is influencing the structural and magnetic behavior, in order to make them useful for applications. Among other magnetic powders useful in medical applications, Fe-Cr-Nb-B submicron powders with low Curie temperature proved to be very appropriate for self-regulating magnetic hyperthermia [4]. Here we report our most recent results on the Fe_{67.2}Cr_{12.5}Nb_{0.3}B₂₀ submicron powders produced by high energy ball milling in a dry and wet atmosphere, from glassy melt-spun ribbons precursors. The effect of post-milling heat treatment on the magnetic properties of the powders is also presented. The structural evolution was investigated after each step of the milling process, enabling one to determine the effect of different milling conditions on the production of submicron powders with suitable magnetic properties. Dry milling results in a rapid decrease of the size of the powders in the first 10 h and to the rapid increase of TC to ~180°C. Wet milling in water leads to a more rapid decrease of the size of the powders, but they still remain in the 1–3 μm range even after 10 h of milling. Wet milling in a surfactant, such as oleic acid, gives the best results: the powders are in the submicron range after 48 h of milling, whilst their magnetic properties are kept closely following the ones of the glassy melt-spun ribbons precursor. Following the structural and magnetic characterization, we have developed a protocol for wet/dry mechanical milling of Fe_{67.2}Cr_{12.5}Nb_{0.3}B₂₀ glassy melt-spun ribbons, which allows

the preparation of powders in the range of 10÷25 nm with tailored magnetic properties, mainly the Curie temperature around 40-45°C.

Acknowledgments. This work was supported by the MCID (NUCLEU Program PN 19 28 01 01) and UEFISCDI (Project PN-III-P2-2.1-PED-2019-3442; Contract No. 502PED/2020 and Project number PN-III-P2-2.1-PED-2019-2054, within PNCDI III).

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T10-P: Fabrication and properties of WO₃ films grown by spray pyrolysis for smart windows applications

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Several materials have been used for electrochromic and smart windows applications over the years, the most promising one being tungsten trioxide (WO₃) [1–4].

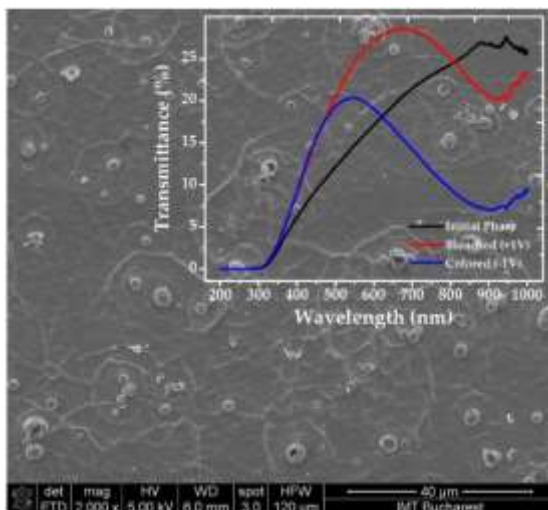


Fig. 1. SEM image of WO_3 film and UV-Vis as inset.

In this research, we present the fabrication and the characterization of WO_3 films, grown onto fluorine-doped tin oxide-coated (FTO) glass substrates using the air carrier spray pyrolysis technique at a deposition temperature of 250 °C. Different volume of precursor solutions were employed, so that the electrochromic performance of the films can be optimized. Scanning electron microscopy (SEM) revealed that all obtained films, are uniform and nanostructured, with a unique surface morphology. Moreover, X-ray diffraction (XRD) analysis showed the presence of the orthorhombic phase of WO_3 . Finally, the influence of the deposition parameters on the morphology of the films as well as the transmittance modification in coloring/bleaching states was studied. An example of the obtained results is shown in Figure 1. Further studies for improving and optimizing the electrochromic performances are ongoing.

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08:00	Plenary Session HALL 1
10:20	Coffee Break
11:00	Plenary & Invited&Oral Session HALL 1
11:00	Invited and Oral Sessions Online
13:35	Lunch
15:00	Invited and Oral Sessions HALL 1
15:00	Invited and Oral Sessions Online
18:05	Coffee Break
18:40	Invited and Oral Sessions

20:25

Dinner

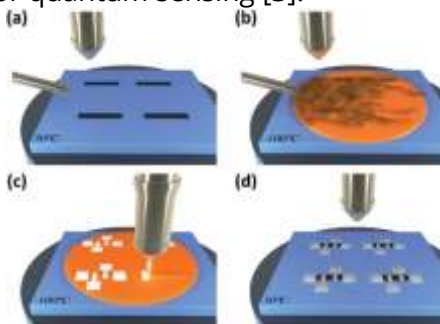
HALL 1

T1-I: Using FIB-SEM equipment to grow unique metallic, magnetic and superconducting nanostructures

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Focused Electron/Ion Beam Induced Deposition (FEBID/FIBID) nanolithography techniques stand out for the growth of functional nanomaterials with high-resolution [1]. In my talk, I will describe three applications of FEBID/FIBID. The first application concerns the use of FEBID for the growth of magnetic tips, with applications in magnetic force scanning microscopy [2]. The second application regards the growth of superconducting nanostructures by FIBID and their potential applications for quantum sensing [3].



Cryo-FIBID process used to grow electrical contacts on 2D materials (e.g., graphene). The third application is based on the use of FIBID under cryogenic conditions (Cryo-FIBID), a new technique that has been applied to grow metallic W and Co deposits, with significant enhancement in the growth speed

and with minimized ion-induced damage (Nanoscale Advances, doi: D1NA00580D).

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T14-PL: Chalcogenide materials development for infrared sensor innovations

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A review of current research on chalcogenide materials contributing to the development of optical sensors will be presented. The 3-15 μm range is a key region for a large number of optical sensor applications in various fields such as biology and medicine, molecular spectroscopy or environmental monitoring. Infrared spectroscopy is a powerful tool for detecting and determining the composition of complex samples. It is a simple, reliable, fast, economical and non-destructive method. In order to further develop this technique especially for on-site real time monitoring, it is crucial to provide suitable infrared materials covering the mid-infrared spectral range. It is in this context that intensified efforts were performed to develop chalcogenide materials that meet the specific requirements for the development of optical sensors dedicated to environmental issues. On the one hand, the

detection of molecules at low concentrations down to a ppm or ppb level is often necessary and Lab-on-chip based on chalcogenide can provide motivating insights. On the other hand, infrared sources are a key entry point for optical sensors. Oxides generate at the best near-infrared light, whereas mid-infrared emissions of 3 to 8 μm are allowed in chalcogenide matrices with lower phonon energy. The down-wavelength conversion mechanism could be adapted in the mid-infrared range to develop incoherent light sources to replace blackbody sources for remote sensing or spectroscopy applications, for example.

Aknowledgement: V. Nazabal is thankful to CNRS, Brittany region, IFREMER and BRGM funds, ANR SEED CGS μ LAB, ANR LOUISE, ANR OPTIGAS and ADEME COPTIK, GACR project (project No. 19-24516S) for financial support.

T9-PL: Emergent magnetic nanoparticles based nanovectors in biomedicine

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¹Laboratory of Advanced Microscopies, University of Zaragoza, Spain

¹Department of Condensed Physics, University of Zaragoza, Spain

Magnetic nanoparticles are considered as promising nanovectors in tumor treatment at the clinic [1,2]. The knowledge of the mechanism triggering the cell dead using magnetic nanoparticles as targeting vectors it is relevant. In particular, the design of this nanovector is fundamental, in order to induce cell death in in vitro experiments. The design will be based on the influence of the physical properties, the applied electromagnetic field [3], magnetic nanoparticles

properties [4], cell lines [5] and internal nanoparticle biodistribution in cells [6]. We report that the tuning of different parameters could lead to suitable procedures in order to trigger the cell death following the apoptosis or necrosis mechanisms. The drastic effect of the intracellular damage induced by magnetic hyperthermia is a key issue for the use of magnetic functional nanoparticles in focused therapies in comparison with exogenous heating [7]. Our results demonstrate that a complex interplay of physical effects in in vitro models makes this technique a very promising alternative or adjuvant therapy for tumor treatment. Consequently the optimization of the functional nanomaterials is relevant for their application. Other field of relevance among the applications of magnetic nanoparticles is the targeted drug release. In this field the use of core@shell nanoparticles becomes relevant. We have investigated the performance of Fe/Fe₂O₃@C due to their biocompatibility and adsorption/desorption properties [8,9].

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T9-PL: Resistive switching devices for memory and computing applications

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Our focus in this presentation is on inorganic materials, namely oxides that are deposited by sputtering and exhibit resistive switching. In these materials the resistance can be changed between a high and a low value by the application of appropriate voltage pulses between two metal electrodes that enclose the oxide. We shall discuss devices made from insulators describing two general material cases. In the first case the resistance modulation is interpreted by the formation of conductive nanofilaments within the oxide due to the removal of oxygen atoms from the lattice while in the second case is due to the diffusion of metal ions from one of the electrodes inside the insulator. We shall then discuss the influence on the resistive switching but also to the uniformity of the behavior of a large number of devices when we embed metallic nanoparticles within the oxides during their growth process. The resistance switching can be used for the realization of new non-volatile memories or artificial synapses

that are needed in neuromorphic computing. The devices presented above will be analyzed with these two application fields in mind [1,2].

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Plenary & Invited & Oral Sessions

HALL 1

T3-PL: Ferroelectric oxides for photovoltaic applications

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Although silicon is nowadays by far the most used semiconductor in electronic devices, oxide materials are becoming more and more appealing because of their wide variety of properties such as transparency, chemical stability, abundance, low cost, reduced toxicity, and versatility of the fabrication techniques. In most cases however, doping is required to address different functions. Oxides can thus be used as transparent conductive materials (e.g. Sn-doped In₂O₃), magnetic semiconductors (e.g. Co-doped ZnO), photon management materials (e.g. RE-doped ZnO), etc. More recently, oxides were found to have a potential interest for photovoltaic solar cells. The main issue related to these oxide materials is

their high band gap which, in order to fit the AM 1.5G solar spectrum, should be lowered to approach that of an ideal absorber in a single junction solar cell (around 1.3 eV).

In solar cells, ferroelectric materials are promising as they can lead to large open circuit voltages, well above the value expected from the band gap width. Moreover, contrary to conventional photovoltaic devices, no p-n junction is needed since the internal electric polarization is now responsible for electron-hole separation. The main challenge is to develop ferroelectric oxide materials with high an appropriate bandgap with respect to the solar spectrum. If oxides such as BiFeO₃ ($E_g \sim 2.6$ eV) were among the first FE materials investigated as possible photon absorber and showed open circuit voltages up to 15 V, the efficiency remains modest mainly because of the small short circuit current. Here we show that by replacing half of the Fe atoms by Cr, in the resulting Bi₂FeCrO₆ (BFCO) double perovskite the gap can be decreased down to 1.5 eV. In epitaxial films, the gap can be modulated by controlling the growth conditions which influences on the Fe/Cr order. Band structure calculations confirmed the experimental results. The ferroelectric properties were studied using the piezoresponse and conductive force microscopy (PFM and CAFM). Finally, test devices based of BFCO were fabricated and their photovoltaic properties will be presented.

T1-I: Formation mechanism of Ge-rich layers on SOI by condensation at different temperatures

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Silicon-Germanium strain engineering has been used for more than two decades in silicon-based devices and has contributed to the scaling down of a transistor's size and to significant improvements in device performance. However, while conventional silicon-germanium based electronics has experienced rapid and steady growth, thanks to this continuous miniaturization of transistors, this trend cannot continue indefinitely. Industry has already moved to alternate methods such as FinFET devices, in which a thin silicon channel is placed vertically, and the FD-SOI (FD-SGOI) design consisting of a thin film Si(SiGe) channel placed horizontally. For nodes scaled down below 28 nm, low power operation will be inherently hindered by both the imperfect interface, non-uniformity of ultra-thin films and quantum confinement effects, which increase the effective bandgap. In these devices, despite the intense research activity on the strained SiGe ultra-thin body, which accounts for a large portion of such microelectronic devices (below the 45 nm node), we still fail to properly understand the mechanisms that limit hole and electron mobilities in SGOI layers. In addition, one of the main challenges for Si based devices remains the fabrication of efficient group-IV photon sources/photon detectors compatible with the microelectronic industry, which would usefully replace

the integration of III-V heterostructures on Si. The major bottleneck is that group-IV semiconductor elements have indirect bandgaps, but with possibilities of being transformed to direct bandgaps using strain engineering strategies.

In this presentation, we will review the formation mechanism of Ge-rich layers on SOI by condensation at different temperatures. TEM cross-section and GPA analysis of the heterostructures will be presented. We will also report the physical and optical properties of these heterostructures. Special attention is devoted to the influence of the SiGe thickness reduction (up to few MLs), where quantum confinement is prominent in the optical properties of the layers. Raman and PL results will be presented to better explain such confinement behavior. We show that novel SGOI substrates could represent a key strategy for the fabrication of future photonic devices.

T1-I: Atomic Layer Deposition of ultrathin conductive silver films

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Silver presents a low electrical resistivity at low thickness, a high reflectance on visible-infrared spectra and a low thermal conductivity. It is used in a large range of applications, either as nanoparticulate (NP) films (in devices based on localized surface plasmon resonance) or as continuous thin films for highly reflective optical mirrors or as infrared reflecting coatings. Atomic layer deposition (ALD) is known for its ability to produce

an accurate and precise thickness control giving uniform and conformal film growth thanks to the sequential and self-limiting surface reactions of precursors. However, the intrinsic Volmer-Weber growth mechanism hinders the synthesis of ultra-thin continuous Ag films as it favors islands morphology rather than continuous one.

After a careful investigation of the Plasma Enhanced (PE)-ALD parameters and their impact on the Ag deposition, we prove the self-saturated regime required for obtaining good control of the deposition and large-scale uniformity. An empirical model which explains the silver NPs growth mechanism correlated with the experimental results obtained is also proposed. This fine control of the Ag NP morphology is of a great interest for applications requiring precise NP dimensions. Moreover, we present an original two-step PECVD-CVD synthesis method that might be more promising for obtaining the challenging continuous and highly conductive ultra-thin films deposition. The first step provides a uniform new morphology made of compact Ag NPs that is usually not achieved at low thickness with CVD or ALD. The experimental results suggest that the chemical reaction occurs not only on the surface but also in the gas phase. The second step, consisting in plasma post-treatment enhances the electrical conductivity of silver films by increasing the connectivity between particles. Electrical performances comparable those describing films obtained by PVD are achieved (critical thickness as low as 15 nm and an electrical conductivity of 3.9×10^5 S/cm for a 40-nm thick Ag film). The method can also be extended to other noble metals, in particular copper and

gold, for which the deposition using chemical vapor-based methods is a very active field.

The novel two-step approach leads to a high film conformality on complex lateral high aspect ratio structures (LHAR with AR of 100), with better coverage than the one reported up to now for ALD of Ag. The study of the optical behavior of Ag films gives information about their morphology. The presence of an absorbance peak in the visible range is a signature of metallic NP morphology causing localized surface plasmon resonance. By following the film reflectivity spectrum of Ag NP films, a 'continuous-like' behavior explained by the Drude model is found at low wavelengths whereas higher wavelengths highlight a 'particle-like' behavior sticking to the oscillator model. This evolution is similar for separated NPs using standard PE-ALD and for the films fabricated using the new approach. The plasma post-processing gives strong increase of the infrared reflectance (up to 97%) and a strong decrease of near infrared transmittance (as low as 3% for a 40-nm-thick film).

T1-I: Nanoelectronic Devices based on spin molecular spin crossover materials

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Switchable molecular compounds are being more and more considered for the replacement of conventional inorganic semiconductor materials as the miniaturization of silicon based devices approaches fundamental technological and physical limits [1]. While early developments with molecular switches focused primarily on single molecule device, [2] the recent progress of “organic electronics” [3] has paved the way for considering the use of molecular switches in more conventional devices as well, such as field-effect transistors, light emitting diodes, spin valves, etc.

In this presentation, we present a comprehensive review of our research on charge transport properties of spin crossover complexes. This includes both the effect of spin-state switching on the dielectric permittivity and electrical conductivity of the material and vice versa the influence of an applied electrical field (or current) on the spin-state of the system. The survey covers different size scales from bulk materials [4,5] and thin films [6,7] to nanoparticles [8] and embraces the presentation of several device prototypes and hybrid materials as well.

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T3-O: Ultrasound synthesis of rare-earth modified TiO₂: effect of rare-earth element on TiO₂ structure and its photocatalytic activity

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In order to increase the performance of titania photocatalyst, modification with rare-earth elements is considered as one of the possibilities to narrow its band gap [1,2]. The aim of this study was to find the effect of introduced various rare-earth elements in the synthesis of titania on its structural, optical, morphological, and photocatalytic activity. TiO₂ was synthesized using titanium isopropoxide as titanium source via ultrasound synthesis procedure and modified with La, Sm, Gd, and Dy, allowing to fine tune the textural, structural, and morphological properties of titania, in a short time. Physical and chemical properties of the synthesized samples were investigated by N₂-sorption, XRD, SEM-EDX, FT-IR and UV-vis DR techniques for a better understanding the effect of the used rare-earth elements. As well, the photocatalytic activity has been found to be improved, as a result of physico-chemical modification of titania by one-pot ultrasound-assisted synthesis method.

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T3-O: Insights into some organic light-emitting materials based on a donor-acceptor system for OLEDs

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Organic light-emitting diodes (OLEDs) attracted large interest in the last decades due to their perspective application in flat-panel displays, but also as one of the next-generation light sources. OLED devices demand less energy for light emission compared to older light sources, although they still need improvements to get more efficient [1]. Small organic molecule and polymer materials are among the most used constituents of OLEDs. As active layers, they must obey some important characteristics, such as high quantum yield of luminescence in film state, efficient n and p carrier mobility and good colour purity besides ability to form defect-less films with good thermal and chemical stability [2]. Since the efficiency and stability of OLEDs are still challenging, further work is necessary to develop new light-emitting organic materials. One strategy to tune the colour of the emitted light consists in the employment of donor-acceptor systems endowed with intramolecular charge transfer features [3]. They have the great advantage that both the electron donor and the electron acceptor can contribute to charge-transfer absorption and

emission enhancement, while hole and electron carriers can be nearly balanced. However, these molecules possess an extensively π -conjugated structure, therefore are prone to aggregation in solid state through intermolecular π - π interactions and can behave as weakly emissive or even nonemissive. To prevent the light-emission quenching, doping of an efficient emitter into a suitable host as a polymer matrix is frequently used. Here we present our attempts to develop a donor-acceptor organic molecule with variable fluorescence in solution which is able to emit pure light in solid state. Besides a detailed characterization with regard to the structural, photo-optical and electrochemical features, this study focuses on its light-emitting performance as both non-doped solid emitter and dopant in a polymer matrix.

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T3-O: Proton conductive membranes for fuel cells: challenges when cellulose replace nafion

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Fuel cells have a great affinity for renewable sources and modern energy carriers (i.e., hydrogen) for energy security and sustainable development. The electrolyte membrane is deemed a key component for the operation of fuel cells and is used as separator material between anode and cathode. Nafion membranes exhibit high proton conductivity at temperatures below 90 °C, and high humidity, good chemical and mechanical stability, Nafion representing nowadays, the standard proton exchange membrane in fuel cell technology, operating in low temperatures range. However, Nafion fabrication is a costly process, and its utilization at higher temperatures is ineffective. We used three N-containing heterocycles, namely: 1-hydroxybenzotriazole (HBT), imidazole (IM), and 7-azaindole (AI) as dopants for oxidized cellulose. Following dielectric measurements, the highest proton conductivity ($1.2 \cdot 10^{-2} \text{ Sm}^{-1}$) was found for the hybrid material containing HBT, as compared with $2.6 \cdot 10^{-3} \text{ Sm}^{-1}$ for the composite containing IM.

Schematization of the cellulose acetate conversion to cellulose and oxidized cellulose, and visual appearance of the hybrid membranes made from various cellulosic supports with 1-hydroxybenzotriazole (HBT).

In our present study, different cellulose types were used as supports for embedding heterocycles (added in different quantities), and the conductive behavior of the resulted materials was assessed. As a dopant, we opted for HBT, because in our previous study, HBT provided the best values of

proton conductivity. Figure 1: Schematization of the cellulose acetate conversion to cellulose and oxidized cellulose, and visual appearance of the hybrid membranes made from various cellulosic supports with 1-hydroxybenzotriazole (HBT). Acknowledgments. This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE-2020-0476, within PNCDI III.

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Invited and Oral Sessions

Online

T6-O: Statistical analysis of likelihood of donor-induced quantum dots in Si nano-transistors at different concentration

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Silicon (Si) transistors have been the backbone of the electronics industry for decades and have been continuously scaled down into the nanometer-regime (with dimensions on the order of 10 nm). As Moore's law [1] approaches its end of the road, new mechanisms and concepts are studied for low-power, highly versatile devices. In this sense, the individuality

of impurities (dopants) in nanoscale offers an opportunity to study transport of electrons one by one via one (or a few coupled) dopants [2,3], e.g., phosphorus (P) donor(s), working as quantum dots (QDs). This is the basic concept for a new field coined as dopant-based electronics [4]. In this study, we explore statistically the likelihood of the formation of such donor-induced QDs in a range of doping concentrations, below and above the metal-insulator transition for Si (for bulk, $\sim 3 \times 10^{18} \text{ cm}^{-3}$). We show that single-donor QDs are expected in the regime of $N_D \approx 1 \times 10^{18} \text{ cm}^{-3}$ (when the inter-donor distance is $\sim 10 \text{ nm}$). In a few devices, however, it can be expected that double-donor “molecules” can work as QDs. On the other hand, in a high-doping regime of $N_D > 1 \times 10^{20} \text{ cm}^{-3}$ (when the inter-donor distance is $\sim 2\text{-}3 \text{ nm}$), QDs can be formed by a relatively large number of coupled P-donors, while it is rather difficult to preserve the isolation from leads. The statistical analysis can be correlated with experimental results obtained for nanoscale silicon-on-insulator (SOI) transistors doped in different regimes of concentration. Acknowledgement: This work was partially supported by a Grant-in-Aid for Scientific Research (no. JP19K04529) from the Ministry of Education, Culture, Sports, Science, and Technology (MEXT), Japan

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T6-O: Study of Si/SiO₂ core/shell Quantum Dots produced by Pulsed Laser Deposition

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Si/SiO₂ core/shell Quantum Dots (QDs) were produced by pulsed laser deposition method in order to obtain the nanoparticles for application in optoelectronics, solar-cells and even in biotechnology and biomedicine. Silicon has interest for a lot of application because of their biocompatible advantages, namely it is low-cost, inert, abundant and nontoxic. Moreover, the Silicon Quantum Dots (Si QDs) are described in literature that it possesses remarkable proprieties of photoluminescence, like as the band gap tunable emission, the fluorescence lifetime is long. For more efficiencies of wavelength tunable emission, the Si QDs is necessary to be coverage with silicon oxide (SiO₂). For medical application, for minimizing the toxicity of the nanocrystals, it can be coated with organic substances, such as keratin. The Quantum Dots will be also fabricated on the quartz plate. In this work will be present the procedure of preparation of Si/SiO₂ QDs and for investigation of proprieties of these nanoparticles will be used Light Induced Fluorecence (LIF), Fourier Transformation Infrared Radiation (FTIR) and Scanning Electron Microscopy coupled with Energy Dispersive Spectroscopy (SEM-EDS).

Keywords: Si/SiO₂ Quantum Dots, core-shell, keratin, quartz, PLD method.

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T6-O: TiO₂ P25/Fe₃O₄/γ-Fe₂O₃ photocatalytically active nanocomposites and the ecotoxicological effects of TiO₂ P25 on the *Lasius niger* ant species

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Titanium dioxide is without doubt one of the most researched semiconductors in the field of heterogeneous photocatalysis, and even so, there is always a new way to approach this versatile nanomaterial. The current study discusses two main issues of commercial TiO₂: the separation and recycling of the photocatalyst following the wastewater purification process

and the ecotoxicological effect of the material on living organisms.

The present research modified the traditional co-precipitation synthesis method of Fe_3O_4 nanoparticles [1], using only Fe^{2+} precursor and introducing P25 TiO_2 into the synthesis solution, in order to obtain $\text{TiO}_2/\text{Fe}_3\text{O}_4/\gamma\text{-Fe}_2\text{O}_3$ composites. To inspect the composition, crystallinity and morphology of the samples, X-ray diffraction, Diffuse reflectance spectroscopy, Scanning Electron Microscopy with Energy Dispersive Spectroscopy and Raman spectroscopy were employed. Combining TiO_2 with magnetic iron oxide nanoparticles led to a stable, effortlessly removable and recyclable composite with good photocatalytic properties, which were confirmed by the removal of paracetamol from aqueous solution, under UV_A irradiation.

Although P25 is a recyclable photocatalyst, its incidental or direct release into natural ecosystems is inevitable. The second part of the presented work studies the influence of TiO_2 on the food foraging behaviour of *Lasius niger* ant species. Ants were chosen as experimental species due to their global spread and complex social and cooperative behaviour. They use a wide range of trail pheromones for foraging, all of them consisting of different organic compounds. To complete the results of the classical ecotoxicology tests and to search for an explanation of the changes in the *Lasius niger* behaviour after contact with TiO_2 P25, some of the above-mentioned trail pheromone components' aqueous solution, such as 2,5-dimethylpyrazine [2], were treated by photocatalytic degradation under UV_A irradiation in the presence of TiO_2 P25 photocatalyst.

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T6-O: Pt free counter electrode for DSSCs based on reduced graphene doped and codoped with heteroatoms

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The counter electrode (CE) is a key component in Dye Sensitized Solar Cells and has a significant influence on both the photovoltaic performance and the device cost. Platinum is preferred catalyst used for CE because of its high conductivity and good catalytic activity for electrolyte regeneration, as well as good stability. However, it is the most expensive component

of DSSC. For that, there is a need to explore Pt-free materials for the CE in DSCs.

Owing to unique properties, graphene is a promising material to replace Pt in DSCs. However, the lack of intrinsic bandgap and catalytic abilities seems to greatly limit the practical applications of pristine graphene [1].

Many studies and recent review articles have demonstrated that doping can tailor graphene properties by interacting molecules, which either donate or withdraw free electrons, which results in changes to the carbon sp^2 lattice [2]. This affects graphene's surface, chemical, and electronic characteristics, as well as its free charge carrier densities and electrical conductivity [2]. Increases in the amount of defects and/or functional groups do, in fact, contribute to an increase in electrocatalytic activity [3].

The aim of this research is the preparation and characterization of nitrogen and boron mono-doped and co-doped reduced graphene oxide (rGO) as a Platinum free catalyst for CE in DSSCs. The boron and nitrogen co-doping of rGO is achieved by reduction of graphene oxide (GO) with urea and acid boric. The successful preparation of the doped rGO is confirmed by Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), Scanning Electron Microscopy and Transmission Electron Microscopy.

Both XPS and FTIR analyses confirm the presence of different functional groups such as N-H, C=C, C=N, C=O, B-C and C-O. The XRD and Raman spectroscopy were employed to confirm presence of structural defects created by boron and nitrogen

doping of GO. Raman spectroscopy proved that the I_D/I_G values of N-rGO (0.50), B-rGO (0.84) and BN-rGO (0.87) are higher than those of GO (0.44), implying that the heteroatoms were effectively incorporated into the graphene planar layers and more defect sites were formed by heteroatom doping. The XRD analysis shows that the addition of N and B in GO structure caused shifting of (002) diffraction line at $2\theta = 23.13^\circ$ and the calculated d -spacing of NB-rGO is found to be lower than that of GO, indicating the successful incorporation of B and N atoms into the GO layer.

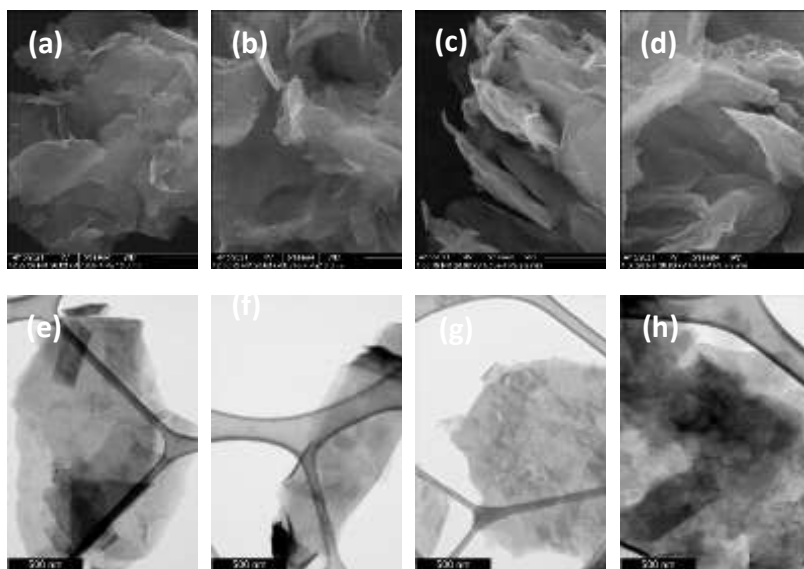


Fig. 1. SEM images of (a) GO, (b) N-rGO, (c) B-rGO and (d) BN-rGO; TEM images of (e) GO, (f) N-rGO, (g) B-rGO and (h) BN-rGO.

The SEM and TEM inspections of doped rGO (Fig. 1) revealed typical laminated structures composed of planar sheets with wrinkles and corrugations.

The electrochemical properties of the doped grapheme materials were investigated using Cyclic Voltammetry and Electrochemical Impedance Spectroscopy. The synergetic effect associated with the B and N co-doping provided rGO samples with better electrocatalytic activity, which is promising for application as an efficient metal-free electrochemical catalyst for CE in DSSCs.

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T6-I: Nanoscale absorption spectroscopic mapping of two-dimensional materials and heterostructures grown by chemical vapor deposition

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Transition metal dichalcogenides monolayers are attracting extraordinary attention for its intriguing optical, electronic and mechanical properties. One of the advantages of this class of 2D semiconductors, with respect to graphene, is the indirect-to-direct bandgap transition as a function of the thickness. In this work we develop Quantitative Nanoscale Absorption Mapping (QNAM)[1], a novel non-destructive and non-contact technique for the analysis of the absorption properties of 2D materials at the nanoscale, developed in collaboration with Attolight AG (an EPFL based company). The technique is based on the cathodoluminescence of the underlying substrate and the concurrent optical absorption of the 2D materials. The electron probe allows to overcome the light diffraction limit and analyze 2D layers with nanometer spatial resolution.

Fig. 1. Sketch of the working principle of the QNAM technique. The QNAM technique can employ standard growth substrate of transition metal dichalcogenides, as oxidized silicon and sapphire. In particular, the defect related emissions of the different oxide provide different spectral range of analysis from UV to the NIR. In particular, we studied the absorption properties of single MoS_2 and MoSe_2 monolayers and heterostructures, demonstrating that the van der Waals heterostructures present an enhanced absorption thanks to the interlayer excitonic interactions. The possible employment of such technique has been enlarged studying the absorption properties of MoS_2 three dimensional pyramidal structures.

T5-I: Doped silica glasses for remote ionizing radiation dosimetry

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Optically activated glasses are essential to the development of new radiation detection systems. Among these systems, optical fiber sensors attract a huge interest due to their small size, intrinsic immunity to electromagnetic interferences, flexibility and ability to be remotely interrogated. They also offer high spatial resolution of the measurement with the possibility to work in hazardous, narrow and constrained environments. In the domain of radiation dosimetry techniques, the application of optical fibers started with thermoluminescence (TL), and followed by radiation induced attenuation (RIA), optically stimulated luminescence (OSL) and radioluminescence (RL). For RL based techniques, the scintillation signal from the radiation exposed probe can be recorded, allowing real-time dose-rate measurements, which makes this technique very interesting for applications in medical or severe environmental domains.

In this talk, results concerning both single Ce^{3+} - and Cu^{+} -activated silica glasses will be presented. Indeed, Ce^{3+} - or Cu^{+} -doped glasses present visible luminescence, under UV or X-excitation, peaking in the blue and green spectral domains, respectively. Based on these optical activities and their ability to tailor the shape and size, efficient copper or cerium-doped silica glasses were used as scintillating material in a remote optical fiber-coupled dosimeter, sensitive to X-rays through both radioluminescence (RL) and OSL processes. As an example, we can mention results related to an optical fiber fabricated from Ce^{3+} -activated silica glass. The optical activity of this fiber was exploited for X-ray radiation dosimetry in a remote all-fibred configuration. The RL signal displays a linear behavior versus the dose rate, at least in the $[330 \mu\text{Gy}(\text{SiO}_2)/\text{s} - 22.6 \text{ Gy}(\text{SiO}_2)/\text{s}]$ range, namely covering five decades. These results reveal the potential of such a fiber, used as both active and guiding material, for real-time remote ionizing radiation dosimetry.

T2-I: Atmospheric pressure plasma synthesis of carbon nano-flakes

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Plasma and laser assisted deposition represent appropriate techniques to synthesize (nano)particles, films and coatings

based on various elements or compounds, with multiple applications in environmental sciences, human health, engineering, technology, and laboratory astrophysics. (Nano)particles with complex organic architectures are emphasizing complex chemical structures, with a variable (poly)aromatic and aliphatic character [1,2]. Among plasma deposition methods, atmospheric pressure plasma deposition of carbon and silicon based coatings, are recently studied mainly due to their flexibility in operation. Dielectric Barrier Discharge (DBD) is a relatively new method for deposition of hydrogenated amorphous carbon (a-C:H) products, very few reports being dedicated to this topics. In fact, compared to the materials deposited using other methods (e.g. mechanochemical synthesis, condensation, physical vapour deposition, plasma deposition, combustion and pyrolysis, pulsed laser deposition), the physical and chemical properties, as well as the microscopic aspects of DBD analogues are remarkably different [4,5]. In this lecture we will present our results on the synthesis and characterisation of carbon nano-flakes, using the DBD in helium (85%) – hydrocarbons (15%). The substrate used in flexible graphite and the particles might be detached from substrate for further analyses: FTIR, XPS, optical microscopy, SEM. Based on spectroscopic data, CH_2/CH_3 ratio, H/C ratio and sp^2/sp^3 ratio are calculated using various methods, while the results from microscopy techniques are used to emphasize the hierarchic organization of particles. At nano scale, the TEM observations, correlated with calculation from micro-Raman spectroscopy reveals the existence of graphene like structures surrounded by a hydrogenated

amorphous carbon phase. The properties of these carbon nano-flakes are allowing us to use them as analogues for dust in space and to study the energetic processing of diffuse and dense clouds.

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T2-I: Laser-generated transient carbon plasmas: peculiar dynamics evidenced by optical and electrical measurements

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Carbon plasmas produced by laser ablation have important applications in PLD of nanostructured materials of high current interest, such as nanotubes, nanowires, graphene, etc. Understanding the fundamental aspects of such transient plasmas in various experimental configurations is useful for optimizing the deposition process. We report here a comprehensive study on the dynamics of excimer laser produced carbon plasmas, including fast ICCD imaging, space- and time-resolved optical emission spectroscopy, Faraday cup ion current measurements, ablated crater depth profiling. A peculiar V-like shape of the emitting plume was evidenced [1]

and explained by the interaction of three plasma structures originating in distinct irradiance areas of the laser spot on the target. The interaction of these structures is also thought to favor an enhanced carbon dimer production, mainly through three-body recombination [1,2], at distances significantly higher than previously reported in the literature, which can find technological applications for the efficient deposition of high-quality carbon-based nanostructures. Using Ar as background gas, the increased collision rate allows extended (both spatially and temporally) spectroscopic investigations of the low-emitting axial region of the unusual V-shape transient plasma [1]. The enhancement of the dimer formation in the lateral structures is confirmed and even amplified using background gas. Furthermore, temperature and electron density values have been estimated from the spectroscopic data, providing additional proofs for the validity of the plasma dynamics scenario built for this unusual plume shape. The carbon ions were also studied by using an electrostatic energy analyzer: the ion current gains a multi-peak structure that is assigned with different types of ions and plasma structures [2]. The physical mechanisms of the separation process are discussed. Finally, we present the first observation of oscillations in the ionic and electronic currents at long distance (17.5 cm) from the ablation target [3]. An original signal processing approach based on the short-time Fourier transform allows unveiling fine details on the temporal evolution of the oscillation frequencies.

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Invited and Oral Sessions

HALL 1

T10-I: Pulsed laser deposition for growth of amorphous chalcogenide thin films

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Amorphous chalcogenide thin films are due to their remarkable optical properties such as wide transmission window, high (non)linear refractive indices and photoinduced phenomena considered as semiconducting materials with different applications in the field of infrared waveguides, all-optical processing components, non-volatile phase-change memories, sensors, etc. This work summarizes recent results in the field of application of pulsed laser deposition for the amorphous chalcogenide thin films' growth. This deposition technique is promising for chalcogenide thin films fabrication due to its simplicity, easy control of the deposition process, and often stoichiometric material transfer from the target to the films. The attention is given to the fabrication and characterization of single layers, but (nano)multilayered structures are also discussed. The photoinduced phenomena in pulsed laser

deposited chalcogenide thin films are depicted. The phase-change materials prepared by pulsed laser deposition are described as well.

T10-O: Developments in functional materials for energy-efficient thermal comfort

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Materials with potential to control the heat flux and to provide energy-efficient thermal management are important for buildings, electronics and clothing [1]. Inspired by fast color changing capabilities of the mirror comb-footed spider [2] we developed multilayered polymer nanocomposite materials with fast changing reflectance and transmittance for infrared wavelengths. The polymers are synthesized through silicone and styrene chemistry, can be formed as films by sequential doctor blading without volatile organic solvents, and the films are scalable in roll-to-roll process. Infrared video camera measurements demonstrated on-demand control of temperature of objects covered with such films by fast mechanical or electrical actuation (<1 second) of the films, with

modulation of heat flux $>100 \text{ W/m}^2$ by synergistic changes in the reflectance, transmittance and absorbance of infrared radiation as effect of applied actuation. Globally, energy savings of $\sim 3\%$ of total energy consumption could be achieved by integration of such materials for buildings thermal management.

Acknowledgments: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P2-2.1-PED-2019-1885, within PNCDI III.

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T10-O: Synthesis and characterization of magneto/plasmonic $\text{CoFe}_2\text{O}_4@ \text{SiO}_2@ \text{Au}$ with biomedical applications in biosensing and bioseparation

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Magneto/plasmonic nanoparticles can combine plasmonic and magnetic properties in multifunctional single structures that exhibit new biomedical applications in such cases as biosensing and bioseparation. Core-Shell nanostructures have generated

immense interest because of their capability to combine both core and shell properties giving rise to new proprieties with vast range of potential applications. Unique phases $\text{CoFe}_2\text{O}_4@\text{SiO}_2@\text{Au}$ core-shell nanoparticles have been successfully synthesized through the Polyvinylpyrrolidone assisted hydrothermal method (CoFe_2O_4 – core) followed by a two-step wet chemical deposition (first SiO_2 followed by Au – shell). Transmission electron microscopy (TEM) images reveal the formation of “raspberry-like” CoFe_2O_4 core particles with an average particle size of 64 nm and average crystallite size of 14 nm. Crystallite size was also calculated with Debye-Scherrer equation on the X-ray Diffraction pattern giving an average size of 19 ± 1 nm. The small crystallite size lead to a small coercive field when compared to highly crystalline CoFe_2O_4 with the same diameter, as shown in the study of the magnetic properties. After the shell deposition, X-Ray diffraction patterns reveal the presence of both CoFe_2O_4 and Au phases in all core-shell samples. The results from X-Ray diffraction are confirmed by TEM images which show core-shell nanoparticles with a gold shell composed of small Au crystallite particles. The Au shells were shown to have a geometry ranging from spherical, in the case of small quantities of gold to highly irregular in the case of excess gold. Energy Dispersive X-Ray Spectroscopy (EDX) mapping was also used in order to investigate the spatial distribution of the component elements inside the produced nanoparticles re-confirming the presence of gold on the surface. The intensity of the Surface enhanced Raman scattering (SERS) effect was tested on the $\text{CoFe}_2\text{O}_4@\text{SiO}_2@\text{Au}$ nanoparticles by using different target molecules.

T10-I: Nanostructured Composite Paints for Electromagnetic Shielding

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This work is related to materials for protection of the human health and the performance of electronic equipment from the harmful effect of the high frequency electromagnetic radiation (EMR) – Fig.1.

The World Health Organization (WHO) has recognized the EMR of smartphones as a potentially carcinogenic agent for people. This is quite important, especially now due to the 5G communication systems, which operate at super high frequencies up to 100 GHz. Such systems, especially their broadcast antennas, may pose a high risk of cancer, reproductive disorders, memory, cellular stress as well as neurological and mental disorders. *The effect of EMR is especially dangerous for children of preschool and school age.* It is also necessary to note the significant impact of EMR on electronic equipment. This is related to a well-known problem of providing the so-called "electronic compatibility", when simultaneously operating different electronic equipment interfere with each other.

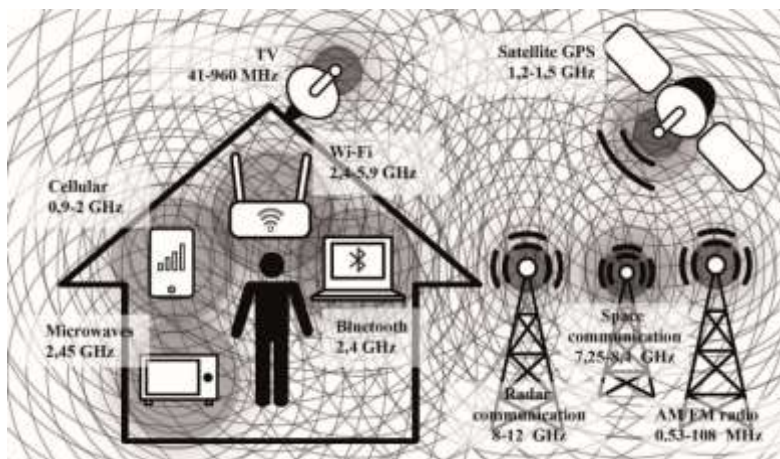


Fig. 1. The main sources of EMR in our everyday life.

A joint team of Ukrainian, Greek and Romanian scientists has developed few types of composite carbon-polymer based coatings in the form of paints for EMR shielding. These paints use mainly carbon fillers of different structure and morphology (graphite, graphene, carbon nanotubes, carbon fibres, graphitized carbon black, etc.), as well as water-based (polyacrylate) and non-aqueous (polyvinylbutyral) polymer matrixes.

The developed water-based composites can be used mainly for interior decoration, formation of electromagnetic screens, thin gradient coatings to protect people in the building from EMR in the microwave range.

The developed composites on a non-aqueous basis have already found a practical application for the electronic equipment, for example, thermal scanners and optical sights. Applying a layer of 150-200 microns on the inner surface of such devices can solve the problem of electronic compatibility and overcome electromagnetic interference.

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Programme, grant G5477 “Nanostructured composite paints for electronics electromagnetic shielding”.

T2-I: Tailoring pulsed laser deposition of p-type semiconducting nanomaterials by in situ plasma diagnostic techniques

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In recent years a special interest was given to the development of p-type semiconductors based on metallic oxides (Cu_2O , CuO , AgO) or copper halides (CuBr , CuCl) due to their exceptional optical and electrical properties. In order to understand the fabrication process in the framework of the pulsed laser deposition technique in situ analysis tools (Langmuir probe (LP) technique and Optical Emission Spectroscopy (OES)) [1,2] were implemented for angular, space and time-resolved measurements of transient plasmas generated in Ar or O_2 atmospheres. The work was focused on understanding the inner mechanism of ablation plasma dynamics and how controlling the ionic energy distribution influences the deposition process. For the case of halide plasma distinctive features of the charge time-of-flight traces recorded by unbiased regime of the probe depict a quasi-monoenergetic plasma with a very directional geometry. The time-resolved LP

analysis revealed halide plasmas are defined by a high plasma potential when compared with the oxide ones, which is directly related to the growth mechanism and the nature of the resulting thin film. The metallic oxide plasmas present some complex features of the ionic cloud as seen by unbiased probe analysis as a time-of-flight measurement tool. Each feature corresponds to an ionization state of the of the metallic ions, results confirmed by OES investigations performed along the main propagation axis and discussed in the framework of multiple double layer formation during plasma expansion. Complementary, OES allowed for the spatial and temporal monitoring of visible and UV emission of the plasma. The nature and pressure of each gas influences the emission in a unique manner, which is correlated with the data from the electrical measurements. Thin films were deposited in conditions identical to the plasma diagnostic ones. The films were investigated using a wide array of techniques (XRD, XPS, AFM, SEM, optical transmission, etc.) and revealed a congruent transfer from the target in terms of stoichiometry coupled with a good crystallinity of the films.

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T8-I On the road to bioactive and multifunctional biointerfaces for implant research: a laser-based approach concept

111

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The design, development and engineering of materials for tissue repair, tissue regeneration and tissue engineering imply the need for bioactive, bioresponsive and bioinstructive interfaces, for promoting and enhancing the desired cellular responses. Therefore, the last decades were characterized by the need of using highly interdisciplinary approaches concepts to address the advanced manufacturing and modifying material surfaces to obtain bioactive, antibacterial or bioinstructive functions, Herein, the advantages of laser methods for soft material concepts with appropriate biological and biomechanical properties supporting tissue healing are described, with focus on bioactive and multifunctional tailored biointerfaces for soft and hard implant research.

T8-I: Solid plasmonic substrates for biomedical applications: from early cancer detection to chiral separation

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SERS represents a very promising vibrational technique able to provide specific molecular information that could have a major impact in biomedical applications such as SERS-based early cancer detection and chiral discrimination. SERS requires the presence of a suitable plasmonic substrate able to generate specific, enhanced and reproducible spectra of analytes when using an excitation laser line ranging from visible to near infrared domain. We propose a new approach for the synthesis of a solid substrate using as building blocks spherical silver nanoparticles purified using the TFF method. The capacity of the here proposed Silver Solid Plasmonic Substrate to generate enhanced and reproducible Raman signals has been tested for two biomedical applications: early cancer detection and chiral separation. For the first application blood samples, collected from breast and colorectal cancer patients and controls, have been investigated by means of SERS. The spectra have been analyzed by means of Principal Component Analysis combined with Linear Discriminant Analysis. Our results allowed the discrimination between the healthy donors and the two types

of cancer patients with very high sensitivity and specificity. The very high diagnostic accuracy of more than 89% for both types of cancer, obtained by performing SERS measurements on pristine blood plasma samples, is a direct consequence of SSPSs ability to generate diagnostic relevant spectral information [1,2].

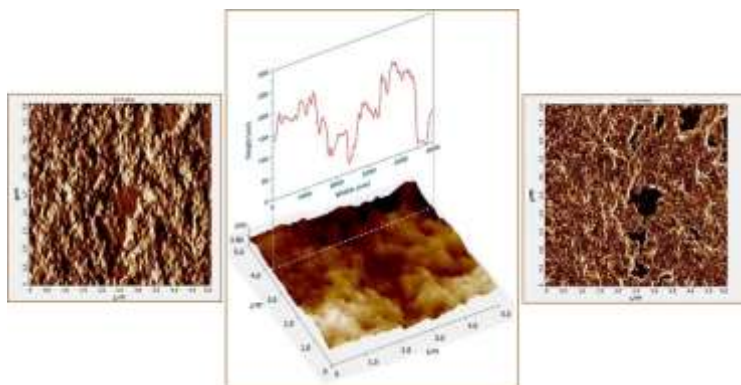


Fig.1. AFM image of the plasmonic substrate

For the second application – chiral discrimination by means of SERS - we present Raman/SERS experimental data that provide useful information concerning the nanoscale interactions between propranolol enantiomers and α , β , and γ cyclodextrins. Raman spectroscopy was used to prove the formation of host-guest intermolecular complexes having different geometries of interaction. The occurrence of new vibrational bands together with a change in the intensities of others are direct proofs of complexes formation. These observations were confirmed by DFT calculations. By performing SERS measurements on our plasmonic substrate

we were able to experimentally prove the nanoscale intermolecular interactions responsible for the discrimination of the two enantiomers.

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T1-O: Charge Carrier Transport in Conjugated Polymer P3HT for Organic Solar Cell Application

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Charge carrier mobility is an intrinsic property, having a strong influence on electronic properties of polymers and determining the conversion efficiency of a polymer-based solar cell. Applying charge extraction by linearly increasing voltage (CELIV) technique [1,2], mobility of equilibrium charge carriers can be determined. In this work, charge carrier mobility of Poly(3-hexylthiophene) (P3HT) polymer thin films was determined by CELIV measurements. The employed technique is based on the measurement of current transients, while a triangle voltage pulse is applied onto a blocking electrode (anode) of a sample structure. Therefore, the equilibrium charge carriers will be displaced to the opposite electrode (cathode), from where they will be extracted [2]. The polymer layers were spin coated on indium tin oxide (ITO) substrates, while the aluminium

electrodes were prepared by physical vapour deposition. Carrier mobility in P3HT polymer was found to be in the range of 10^{-5} – 10^{-6} cm²/(Vs). By increasing the applied voltage, the maximum current transient time is decreasing, because the average velocity of charge carriers depends monotonically on the external field amplitude. In addition, optical and morphological properties were investigated, emphasizing the interdependency between polymer properties.

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Invited and Oral Sessions

Online

T9-O: Preliminary results on biological synthesis of silver nanoparticles using vegetal extracts

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The widespread use of silver nanoparticles (AgNP) in cosmetics, textiles, medicine, pharmacy is based on the antimicrobial properties and the use in optoelectronics, biosensing, etc. is based on the properties of LSPR (localized surface plasmon resonance). The route of all these important amounts of AgNP leads to discharge into the environment where they can interact with vegetation and with some beneficial microorganisms from the biosphere. To reduce the toxicity related to the synthesis, the use and the impact on the environment, we are looking for methods of green chemistry to

replace chemical reducing reagents with natural antioxidants [1]. We present the first data obtained by us in the synthesis of AgNP using green tea extract, lemon juice and blackberry.

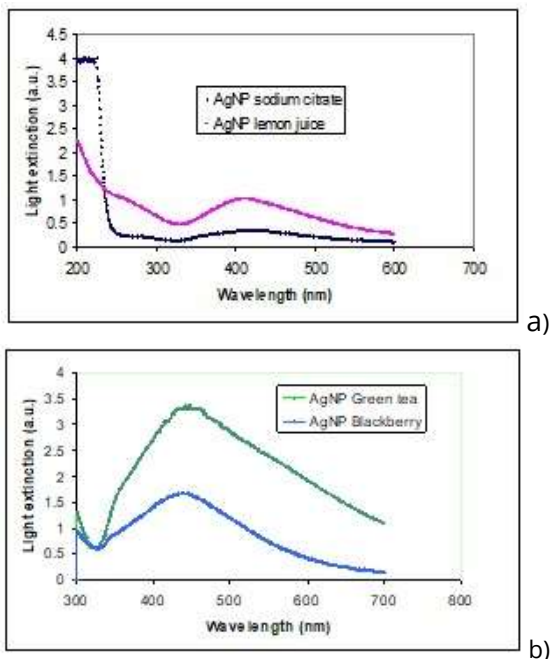


Fig.1. a) Chemical synthesis vs biological synthesis with lemon juice of AgNP; b) Biological synthesis of AgNP with green tea and blackberry extracts

In comparison with the product obtained by the chemical reduction of AgNO_3 with citrate, AgNP reduced with lemon juice leads to a more intense LSPR band, therefore to a higher concentration of AgNP (UV-Vis peak is shifted from 423 nm to 409 nm), (Fig. 1). Green tea and blackberry extracts have led to even higher intensities of the LSPR band indicating a more effective action of natural antioxidants. The position of maximum LSPR is at 437 and 432, respectively (Fig. 2). XRD and

TEM analyzes are expected to complete the study, validating the results obtained by UV-Vis recordings.

Acknowledgements. Part of this research was supported by J.I.N.R. Dubna projects, 2021

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T9-O: Impact of silver nanoparticles obtained by biological reduction on environmental biological indicators

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The production of silver nanoparticles (AgNPs) from bilberry (*Vaccinium myrtillus* L.) fruits extract was studied. The aqueous 10mM AgNO₃ solution when subjected to *V. myrtillus* extract was bio-reduced and ensued in green synthesis of AgNPs. The aqueous bilberry solution was enriched with polyphenols (6.89mg/g gallic acid equivalent) and flavonoids (1.51 mg/g catechin equivalent). The AgNPs synthesis was manifested by a color change from colorless to yellow brown after the introduction of *V. myrtillus* fruits extract. The formation of nanoparticles was monitored spectrophotometrically by measuring the intensity of the surface plasmon resonance band (SPR) of silver. This green procedure has high yields without application of toxic reagents or surfactant template.

As methods of study the AgNPs interactions with environmental biological indicators like microorganism *Phanerochaete chrysosporium*, the biochemical assays of defense systems of antioxidant activity and proteins contents were applied. The lipid peroxidation, expressed as malondialdehyde content has been also evaluated. Overall, results showed a variation of activity of superoxide dismutase and catalase in fungus mycelium depending on the concentration of AgNPs and the age of fungus after inoculation.

T8-O: Nanocomposite formulation to create superhydrophobic surface on wood

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Wood is a favourite material used in many indoor and outdoor applications, because of its abundance, attractive appearance, and easy processing. Even it is a widely used material, due to its structural features and composition its properties are often weakened by its interactions with water resulting in dimensional instability, deterioration of mechanical properties and high susceptibility to biological degradation.

Wood coating is the most common method used for the wood protection against degradation. As coatings, generally, many natural and synthetic materials or mixture between them, solvent or waterborne ones were involved. More recently,

superhydrophobic bioinspired surfaces have attracted high scientific and industrial interest by exploring the superwetting phenomena from nature and by creating composite functional materials by mimicking these biological structures and architectures that cause excellent functions and performance like water repellence, lubricity, self-cleaning, antifouling, anti-icing, antimicrobial effect, corrosion resistance and so on.

In this study, superhydrophobic coatings were successfully produced on intrinsically heterogeneous wood surfaces by a simple, fast and relatively inexpensive impregnation process, and by using silica nanoparticles, a fluoroalcoxysilane and an acrylic polymeric matrix.

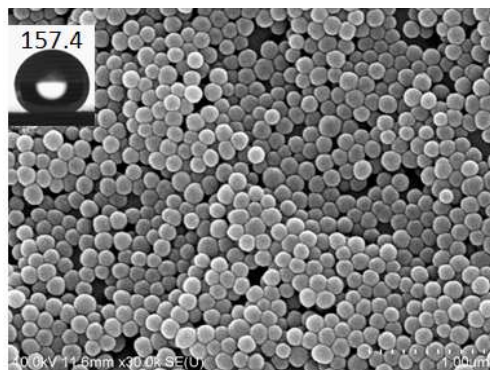


Fig. 1. Surface morphology and the contact angle of treated wood

Pine (*Pinus Sylvestris*) wood pieces were impregnated, and the surface morphology, chemical composition and wetting behaviours were investigated by scanning electron microscopy (SEM), Fourier-transform infrared (FT-IR) spectroscopy and contact angle analyser. Nanoscale spherical particles were uniformly distributed on the different wood surface sections,

providing wood with superhydrophobic properties, as was demonstrated by contact angle measurements (see also Figure 1). The biological resistance was tested against soft-rot fungi. The weight loss of the samples was of about 6%, while the contact angle remained almost constant.

Acknowledgements: This work was supported by the project PN-III-P1-1.1-TE-2019-1375 – Sustainable high-performance coating nanomaterials for bio-based substrates – NANO4BIO.

T8-O: Structural characterization of modified cotton / leather samples using cold atmospheric pressure plasma (CAPP) and TiO₂-SiO₂ - reduced graphene oxide nanopowders by WAXD analysis

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Nowadays, different approaches for modification of textile and leather surfaces (such as application of nanoparticles, irradiation processes, various organic additive coatings etc.) were described in order to develop higher value-added textiles and leather products. This work describes the WAXD – Wide Angle X-Ray Diffraction analysis of surface modification of textile fabrics and leathers using cold atmospheric pressure plasma (CAPP) and TiO₂-SiO₂ - reduced graphene oxide as photocatalytic nanocomposite. The WAXD patterns revealed the typical structure of type I cellulose for cotton and type I

collagen for leather samples. No modification or damaging of cotton and leather surfaces was observed due to the limited depth of plasma treatment, its effects being related to the etching, cleaning or functionalization of surfaces. However, the CAPP and TiO₂-based photocatalytic composites as modifying agents of textile and leather surfaces can add value to textile and leather products. Thus, the optimization of plasma conditions and deposition procedure of photocatalytic particles for surface modification of different textile and leather materials with further experimentation is required.

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T8-O: Post-treatment behavior of atmospheric-pressure plasma treated polymers

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We investigate here the surface modification of polymers treated by an air atmospheric-pressure dielectric barrier discharge (DBD), under conditions simulating continuous processing, with a focus on the dynamics and stability of modified surfaces. The parameters related to the surface energy and the polarity are monitored during post-treatment ageing.

In this respect, polar polymer structures, as poly(methyl methacrylate) (PMMA), polyethylene-terephthalate (PET) and polysulfone (PSU), are tested, in comparison to non-polar polymers, as polyethylene (PE) and polystyrene (PS), in order to evaluate the influence of the polymer structure on the efficiency of plasma surface modification. The selected polymers are offering variety of chemical structure, in terms of

structurally bonded oxygen in their chain, also allowing a comparison between aliphatic polymers, as PE and PMMA, and aromatic polymers, as PS, PET and PSU, known to exhibit enhanced mechanic characteristics and chemical stability, related to intrinsic rigidity and chemical inertness of the aromatic ring.

The water contact angle measured on the polymers after plasma exposure shows a strong increase in the hydrophile character of the surface. Also, the modification of the surface properties is very fast, since the after 0.5 s of plasma exposure the evolution of hydrophylicity levels out.

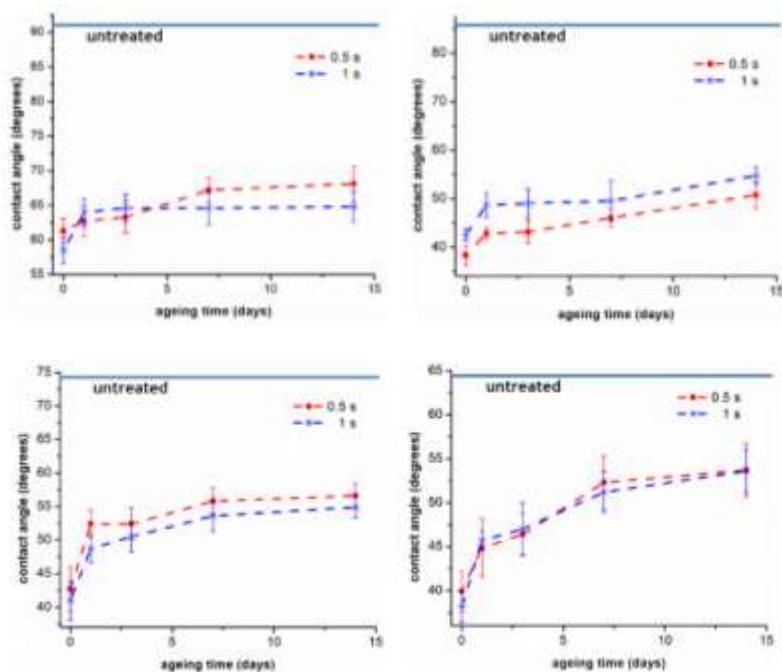


Fig. 1. Post-treatment ageing of plasma-exposed polymers: PE, PS, PET and PSU.

The degree of modification of the hydrophilicity is rendered to evidence by the adhesion work of water W_a , where, interestingly, although the initial value is different for the five polymers, the limiting level of W_a increase is the same for PS, PMMA, PET and PSU.

The treated samples show different ageing behavior (Fig. 1). Although the contact angle remains significantly lower than that for untreated surfaces even after two weeks ageing, in the case of polar polymers, as PET and especially PSU, the recovery is more accentuated than for non-polar polymers, as PE and PS. The parameters related to the surface energy and polarity show again dependence on the chemical structure of the polymers, with the highest stability for non-polar polymers.

We conclude that atmospheric-pressure plasma provided efficient, uniform, and stable surface modification on selected polymers with various chemical structure. The limiting level of modification is similar for all polymers, whereas the post-treatment stability is better for non-polar polymers. Restraining the ageing process is a necessary condition for polymer operational stability.

T8-O: Nanocomposite coatings for wood protection

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Wood is largely used material in different applications, due to its properties and easy processability. However, wood present some drawbacks, like moisture dimensional instability, susceptibility to biological attack, or low UV light stability [1].

Many efforts have been made to increase the life time of wooden products or to improve their properties by thermal and chemical modification of the internal wood structure, impregnation with different chemicals or application of organic coatings able to act as a protecting layer between the external environment and the wood [i.e. 2, 3]. The required properties and therefore the formulation of the coatings depend on their end use and the location of use (indoors or outdoors), but the failure of the coatings is usually due to low adherence of the coating to the wooden material followed by the instability of the underlying wood material.

Recently, attempts have been made to create composite functional materials by using Pickering emulsion polymerisation. Generally, Pickering emulsions have the same basic properties as classical emulsions stabilized by surfactants. The only difference is that in Pickering emulsions the stabilization is done by solid particles instead of surfactants [4].

In the present study we prepared cellulose nanocrystal-reinforced polyacrylate formulation via Pickering emulsion polymerisation to be used for the impregnation of pine and oak wood.

Stable aqueous nanocomposite formulation containing cellulose nanocrystals (CNC) as stabilizing agent and poly butyl methacrylate matrix was synthesized and the effect of the CNC concentration was investigated.

Treated wood samples were analyzed to assess the surface morphology, structural features, contact angle and coating resistance to abrasion and wearing agents.

Acknowledgements: This work was supported by the project PN-III-P1-1.1-TE-2019-1375 – Sustainable high-performance coating nanomaterials for bio-based substrates – NANO4BIO.

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- [2] C.A.S. Hill, *Wood modification – chemical, thermal and other processes*. John Wiley & Sons, Chichester (2006).
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- [4] S.B. Haaj, W. Thielemans, A. Magnin, S. Boufi, *ACS Applied Materials & Interfaces*, 6 (2014) 8263–8273.

T5-O: The contribution of climate and aerosol parameters in the movement of "Saharian smog" over Pelinia, Republic of Moldova

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The presence of air masses containing dust of Saharan origin can cause increases in the levels of suspended particles (PM) in the atmosphere above the limits allowed by the authorities in both large cities and rural areas, directly affecting the health of the population. Globally, the directions of movement of air masses are largely influenced by atmospheric currents, with which they can travel impressive distances, reaching from one side of the planet to another. The present study aims to analyze the direction of movement of the Saharan dust cloud by monitoring meteorological parameters and aerosol characteristics by measurements obtained using the CIMEL Electronique CE318 solar photometer at different wavelengths, which is part of the AERONET network. From the processed and analyzed data, the influence of these parameters was

demonstrated, which favored on May 12th, 2020 the penetration of “Saharan smog” in the Eastern European area, more precisely in the village of Pelinia in the Republic of Moldova. The analysis of meteorological parameters consisted in collecting and centralizing data on wind direction and speed, which showed the important role of meteorological conditions in the movement of air masses containing dust of Saharan origin and it's spread in populated areas both rural and urban. Acknowledgments. This research was funded by Ministry of Research, Innovation and Digitization, project FAIR_09/24.11.2020 and by the Executive Agency for Higher Education, Research, Development and Innovation, UEFISCDI, ROBIM- project number PN-III-P4-ID-PCE2020-0332.

T11-O: Synthesis of freestanding porous alumina and copper nanowires by electrochemical methods

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We report on synthesis of freestanding porous alumina, together with copper nanowires (Cu NWs) fabrication by electrochemical methods, both to be used as targets for high power laser experiments at ELI-NP. Preliminary processes (mechanical polishing, thermal treatment, electropolishing) of the as-received aluminum (Al) plates, used as substrate, were necessary to obtain a smooth and contaminant free surface. Several surface characterization methods and elemental composition techniques have been used in each step of the fabrication process, such as: Scanning Electron Microscopy, Electron Backscatter Diffraction, Energy Dispersive Spectroscopy, optical profilometry and optical microscopy. The

process key-parameters (e.g. temperature, anodization voltage, Al plate lateral dimensions, stirring speed) have been optimized and controlled to obtain the desired characteristics of porous alumina on Al substrate, which was used as a template for Cu NWs deposition. Cu NWs were deposited in porous alumina by DC and pulsed AC electrodeposition method, resulting in NWs of 0.5-10 μm long and 50-200 nm in diameter, on aluminum substrate. The freestanding alumina, obtained after applying the detachment method of stair-like reverse biases, had a thickness that can be varied in the 7-100 μm range, with pore diameter of 30 to 100 nm and 30-100 nm interpore distance. The parameters used in the detachment process (number of stairs and duration of each stair, temperature) have been optimized to result a nearly defect free, freestanding alumina, to be used in laser experiments. The bottom side (barrier layer) of the alumina template was also dissolved, leading to open pores all the way through the target. For laser-driven particle acceleration experiments, both Cu NWs and freestanding alumina templates with or without opened bottom pores are of interest and will be used at ELI-NP facility. The freestanding alumina templates, with lateral dimensions $10 \times 1-2 \text{ mm}^2$, are mounted on a custom-made C-shaped frame on a few centimeters long stalk, on a rotating wheel with 16 positions, placed in the laser experimental area for the intended tests.

T6-O: Non-destructive investigation of the edge and screw threading dislocations in GaN layers

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² *Electron Microscopy Center "Prof. C. Craciun", Faculty of Biology & Geology, "Babes-Bolyai" University, Cluj-Napoca, Romania*

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⁴ *Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, USA*

A major problem in heteroepitaxial layers is related to the strain relaxation processes mainly induced by the difference of the lattice constant between layer and substrate. In the strain engineering context, a quantitative analysis of the emerged structural defects, as well as a deeper understanding of their nature became a highly desirable task for further development of the devices. In this study, structural investigations of the mismatched gallium nitride (GaN) layers grown on SiC, Al₂O₃, and Si substrates were performed using multiple X-ray diffraction techniques. The resulted threading dislocation density evolved from the lattice mismatch was quantified in two independent ways: firstly, using the mosaic block model [1], which takes into account peak width, and, secondly, using the diffuse scattering model, which considers only the tails of the rocking curves [2]. Both models indicated the close relationship between the number of dislocations and the lattice mismatch, which plays a fundamental role in TDs' generation. Also, SEM micrographs support these findings -Figure 1.

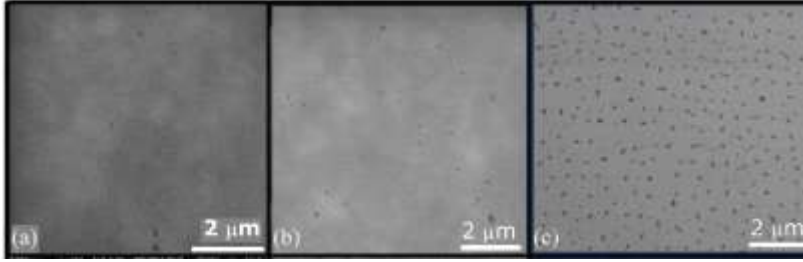


Fig. 1. Top-view SEM micrographs on GaN thin films grown on SiC, Al₂O₃ and Si.

To gain further insights regarding threading dislocations, grazing incidence X-ray diffraction was employed to obtain the absorption profiles of the x-rays, which can provide supplementary information concerning the distribution of threading dislocations along z-axis, as well as about the annihilation mechanisms between adjacent dislocations [3].

[1] Metzger et al., *Philos. Mag. A.* 77 (1998) 1013–1026.

[2] Kaganer et al., *Phys. Rev. B* 72 (2005) 1–12.

[3] Romanitan et al., *J. Alloys Compnd.* 858 (2021) 157723

Invited and Oral Sessions

HALL 1

T4-I: Magnetic and magnetooptic properties of epitaxial Heusler alloys films fabricated by DC magnetron sputtering

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Heusler compounds have composition XYZ (so called half-Heuslers) or X₂YZ (so called full-Heusler). Their tuneability originates from large number of elements. Due to this they are a suitable material class for development of new materials. This provides the opportunity to adjust electronic structure and hence material properties in many desired directions, such as: half-metallic material for spintronic applications, zero-gap topological semiconductors and etc. The properties of Heusler alloy are very sensitive to any non-stoichiometry and crystalline defect. Due to this the fabrication of the films from one single targets in many systems is not very suitable techniques to maintain the structural properties of growth films. In our work we fabricated Rh-Mn-Bi, Rh-Mn-Sb and Co-Ti-Sn systems thin films by direct magnetron co-sputtering from three single elements targets using Ar as the sputtering gas. Deposition is

carried out in an UHV vacuum chamber evacuated before deposition to pressure 10^{-7} Pa. The distance between the targets and substrate was fixed to 10 cm. The angles between the substrate normal and magnetron toruses were 15 deg. For sputtering single elements one inch targets were mounted on UHV magnetron toruses with independent powers supplies. Deviation of composition from stoichiometry becomes a critical problem, especially due to Bi evaporation from surface of the growing films at high deposition temperature. The silicon substrate with diameter of 3 inch was mounted as a substrate to perform the measurements of the composition of the deposited films in this large substrate with the purpose to determine the space distribution of the particular metals deposited from all three toruses. The plasma properties were monitored by optical emission and phase s spectroscopies. The relation between plasma properties and films structured was examined. We focused on the systematic structural characterisation of the fabricated films by XRD, AFM, TEM, XPS, PEEM, ARPES as well as magnetic and magneto-optical characterisations.

T4-I: Magneto-optical spectroscopy applied to systems for organic and inorganic spintronic applications

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The interaction of light with magnetized matter is a fascinating natural phenomenon, which allows to study various physical

properties of the material under investigation. The measurement of the state of polarization of an electromagnetic wave induced by the interaction with a magnetized sample is one of the many possibilities used experimentally. The change in the polarization state induced by reflection on a magnetized sample is known as magneto-optical Kerr effect (MOKE). Spectroscopic MOKE measurements on thin films or layer stacks provide access to the intrinsic magneto-optical properties of the component materials and to the related structural and electronic properties. MOKE spectroscopy has been shown, for example, to be a sensitive tool for the characterization of molecular orientation in organic layers [1,2] as well as for the characterization of the electronic changes induced by crystallization of ferromagnetic layers [3,4]. Furthermore, interface effects occurring in organic/inorganic heterostructures can be revealed by the analysis of the magneto-optical response [5,6].

[1] M. Fronk, B. Bräuer, J. Kortus, O.G. Schmidt, D.R.T. Zahn, and G. Salvan, *Phys. Rev. B*, 79 (2009) 235305.

[2] B. Bräuer, M. Fronk, D. Lehmann, D. R. T. Zahn, G. Salvan, *J. Phys. Chem. B* 113 (2009) 14957

T4-I: Band structure and topological state in Bi₂Se₃ single crystal doped with VIII B group metals

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Topological insulator materials are gaining more and more interest due to their applications in spintronics [1-3]. In this study, bulk single crystal MxBi_{2-x}Se₃ (M = respective metal) (x = 0.02) ternaries were prepared by doping with VIII B (Fe, Ru, Os) group metals. Synthesis of the materials comprised careful thermal processing at almost equilibrium conditions. Doping can be employed for band structure engineering and treatment/control of common defects of the Bi₂Se₃ semiconductor. The selected group of metals have gained only limited scientific attention, unlike Mn for instance. They constitute of a ferromagnetic element and heavy metals with stronger spin orbital interaction. Resulting topological states were experimentally and theoretically analyzed by photoemission and ab initio calculations.

For the photoemission measurements, samples were prepared by in-situ scotch tape exfoliation under ultra high vacuum conditions immediately before the measurement.

E_{binding} vs k_{ll} projections of the reciprocal space were studied. Doped samples were also compared with undoped samples, i.e. natural n-type pure Bi₂Se₃. There are obvious changes both in positions of the Dirac cones on the energy scale and in the

density of states, see Fig. 1. $\text{Fe}_{0.02}\text{Bi}_{1.98}\text{Se}_3$ displays band gap opening with the magnitude of around 0.1 eV.

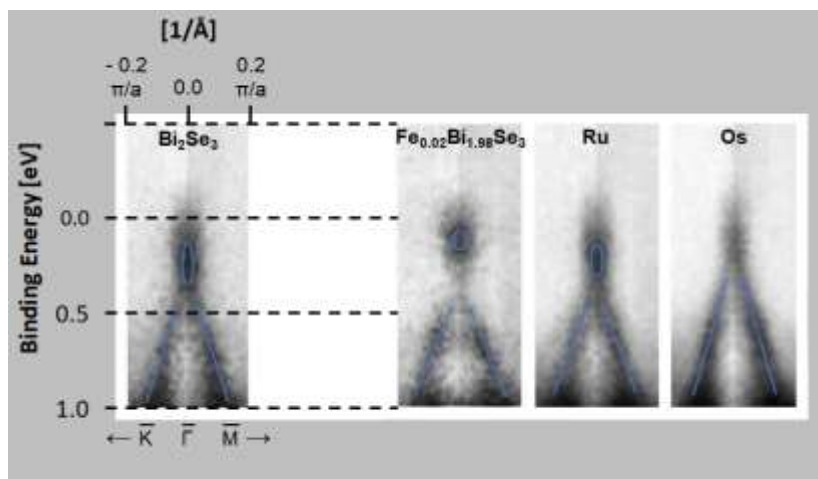


Figure 1. Measured Dirac cone structures. Dirac features and contribution form bulk conduction band are highlighted.

The Ru doped sample exhibits band structure closest to the pure material with a relatively high contribution to the density of states from the conduction band levels. An upward shift is clearly seen at the Os doped sample. In general, the distance between the upper valence states and the Dirac point increases with the dopant element atomic number, as also supported by calculations with dopants substituting Bi.

- [1] J. Sanchez-Barriga et al, PCCP 19 (2017) 30520.
- [2] J. Teng et al, J. Semicond. 40 (2019) 081507.
- [3] J. Sanchez-Barriga et al, Nat. Commun. 7 (2016) 10559.

T4-O: Magnetic Properties of CoFe₂O₄ Nanoparticles

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The magnetic CoFe₂O₄ nanoparticles were prepared through the hydrothermal chemical route. The prepared compounds were found to be single phase. X-Ray Diffraction measurements show that all samples crystallize in the cubic Fd3̄m space group with the lattice parameter $a = 8.38 \text{ \AA}$. The average crystallites sizes were found to be between 11 nm and 18 nm depending on the PVP molecular weight. Transmission electron microscopy images show different tendencies growth depending of the length of the PVP polymer added. It was shown that by using this PVP the morphology of the particles to spherical, cubical and rhomboidal can be tuned. Magnetic measurements performed in an external applied magnetic field between -2 T and 2 T, show small hysteresis loops at room temperature in concordance with the particle size shown on the TEM images. Small coercive fields, H_C , between 300 Oe and 50 Oe were found, the H_C decreasing when the PVP molecular weight decreases. It was shown that the saturation was not attended in 2 T external magnetic field for all samples. The relaxation of magnetization follows an exponential relation $M(t)/M(0) = A \exp(-E_a/k_B T)$. The activation energy E_a is dependent on particle sizes and temperature of measurements.

T4-O Magnetic properties of some iron oxide nanoparticles, nanocomposites, and thin films

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Preparation and properties of iron oxide nanoparticles have been the subject of numerous studies, magnetic materials being highlighted in nanoscience, medicine, and biotechnology. Mesoporous materials and polymer are good matrices for iron oxide nanostructure isolation, allowing the control of size nanostructures and properties.

We present our results regarding the synthesis and structural and magnetical characterization of iron oxide nanoparticles synthesized by self combustion method, iron oxide/MCM-41, iron oxide/silica/polysiloxane nanocomposites and iron oxide thin films deposited by spin-coating.

Electron paramagnetic resonance (EPR), magnetic measurements and Mossbauer spectroscopies were used to study the distribution, the content of iron oxides and the interaction between magnetic nanoparticles.

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|-------|---|
| 08:00 | Plenary Session
HALL-1 |
| 10:20 | Coffee Break |
| 11:00 | Invited and Oral Session
Hall1 |
| 11:00 | Invited and Oral Session
Online |
| 13:35 | Lunch |
| 14:00 | Excursion to Girona |
| 20:00 | Dinner |

HALL 1

PL: Laser-induced graphene from renewable materials

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In the recent years the synthesis of 3D graphene by laser irradiation has emerged as a very promising alternative to conventional technology, mainly due to its versatility associated to a low cost, effective and simple process.

Since the discovery, LIG has attracted intense attention from both academia and industry and found broad applications in areas such as energy conversion and storage, physical sensors, biosensors and desalination.

Laser-assisted process can enable facile, mask-free, large-area, inexpensive, customizable, and miniaturized patterning of laser-induced porous graphene on versatile carbon-based substrates (e.g., polymers, wood, food, cork, textiles) in a programmed manner at ambient conditions.

By combining the high tailorability of its porosity, morphology, composition, and electrical conductivity, LIG can find a broad range of different applications in emerging applications, especially on the flexible ones.

In this presentation, we overview the recent studies of LIG-based biosensors and physical sensors using substrates from renewable origin like cellulose and cork. The applications of LIG in flexible energy generators and photodetectors are also presented. We finalize, by briefly discussing the future challenges and opportunities by these new and stimulating scientific area and some insights to emerging applications.

T6-PL: Femtosecond spectroscopy of excitons and charge carriers in semiconductor quantum dots used in photocatalysis.

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The report is devoted to the study of the dynamics of excitons and charge carriers in quantum dots (QDs) of type II / VI by the method of femtosecond spectroscopy. The talk discusses QDs based on zinc and cadmium chalcogenides, as well as their alloys. Particular attention is paid to QDs doped with Mn or Cu ions. Transient absorption (TA) spectra exhibit the spectral features of excitons and charge carriers. Figure 1. shows transient spectra Mn²⁺ doped QDs.

TA spectra of QDs fabricated from the manganese doped Mn²⁺: Zn_{~0.5}Cd_{~0.5}S/ZnS alloy reveals a specific feature that can be attributed to electrochromic Stark shift of the band-edge exciton. This feature manifests itself as an absorption peak in the TA spectrum appearing at a time delay of about 1 ps. The

delayed rising and decay kinetics of this Stark peak in the manganese doped QDs significantly distinguish it from the known

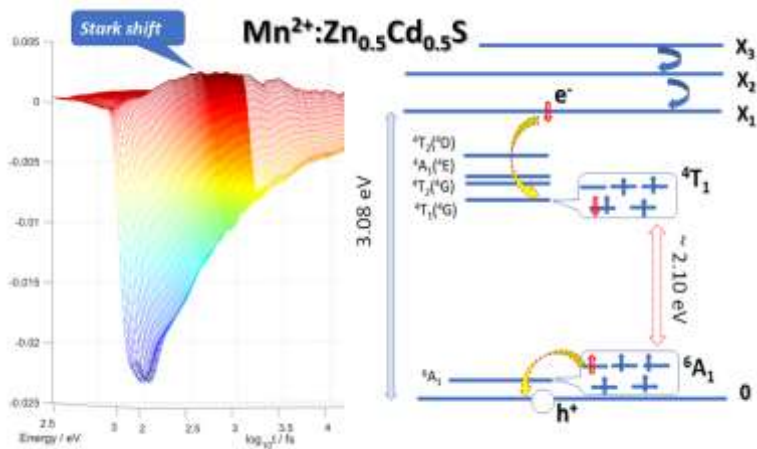


Fig.1 Stark peak associated with electrochromic shift caused by exciton-exciton interactions in undoped QDs at the shortest time delays (left). Femtosecond transient absorption spectra of $\text{Mn}^{2+}:\text{Zn}_{0.5}\text{Cd}_{0.5}\text{S}/\text{ZnS}$ QDs (left). Stark peak evidence the charge transfer. Scheme of charge transfer events leading to the Mn^{2+*} excitation (right).

The comparative kinetic analysis of TA spectra of manganese doped and undoped QDs suggests that the Stark peak in the Mn^{2+} doped QDs occurs due to development of an electric field in these QDs. The delayed appearance of electric field can be explained by the oxidation of Mn^{2+} by holes and the subsequent reduction of Mn^{3+} by electrons from the $1S_e$ state with the formation of excited $\text{Mn}^{2+}(\text{d}^5)^*$ ions. The revealed Stark peak suggests a charge-transfer mechanism of Mn^{2+} excitation by the band-edge exciton, it differs from the non-radiative energy transfer mechanism, which does not imply the development of an electric field in the QDs. The excited Mn can act as a reservoir of excitation energy, which promotes the generation of "hot" electrons involved in photocatalysis. The

talk discusses the problem of relaxation of “hot” excitons, generation of “hot” electrons, and their participation in the photocatalytic reduction of protons to molecular hydrogen.

Aknowledgments. This work was supported by Russian Science Foundation (grant number 17-13-01506).

PL: Silicon-based quantum emitters at telecom frequency

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Quantum Technologies (QT) are poised to disrupt several industries in the next years, by revolutionizing communications (e.g. quantum cryptography), sensing (weak magnetic field, solid state memories) and computation tools (quantum computing), leading to very high productivity gains. Qubits, the building blocks of quantum computing are being implemented in several platforms such as photons, trapped ions, superconductive circuits. Among them, semiconductor-based platforms remain highly appealing as they can in principle allow linking anchored QBs (e.g. spin, charge state) to flying QBs (photons), all while working with an established and well-known material, that constitutes the backbone of the electronics industry. Several structures have been proposed and investigated for flying QBs from solid-state light sources. The archetype of this latter kind of light sources are negatively charged nitrogen-vacancy pairs in diamond (Nvs) [1]. They have an optically active spin-triplet ground state, are well-isolated from the surrounding carbon lattice and have been used in many demonstrations of early quantum devices.

Micro- and nano-architectures based on silicon drove the electronic revolution in the 60's and nowadays represent the dominant platforms for integrated photonics. This is possible thanks to the versatility of this material for carrier transport and to its transparency for light propagation in the near-infrared frequency range. When light emission is concerned, the use of Si-based devices is hindered by the indirect nature of its energy bandgap. However, by exploiting point defects, one can envision light sources in Si and silicon-on-insulator operating at near-infrared frequency.

Here we report the isolation of single optically active point defects in a commercial silicon-on-insulator wafer implanted with carbon atoms forming the well-known G-center (consisting of an interstitial silicon atom bridging two adjacent carbon atoms) [2]. They exhibit a bright, linearly polarized single-photon emission with a quantum efficiency of the order of unity [3]. This single-photon emission occurs at telecom wavelengths suitable for long-distance propagation in optical fibres. Moreover, we show the detection of individual emitters in silicon belonging to six, new, different families of optically active point defects (likely related to carbon). Single photon emission is demonstrated over the 1.1–1.55 μm range, spanning the O and C telecom bands [4]. We analyze their photoluminescence spectra, dipolar emissions, and optical relaxation dynamics at 10 K. For a specific family, we show a constant emission intensity at saturation from 10 K to temperatures well above the 77 K liquid nitrogen temperature.

Our results show that silicon can accommodate single isolated optical point defects (as in wide-bandgap semiconductors),

despite a small bandgap (1.1 eV) that is unfavourable for such observations. Given the advanced control over nanofabrication and integration in silicon, these individual artificial atoms are promising systems to investigate for Si-based quantum technologies.

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T10-PL: Materials Sustainability to Shape Our Future

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Today science is essential to enable comfort and welfare, as well as prosperity to regions and countries. This implies fostering the creativity of scientists and consequent innovations to support the current societal challenges. In this respect, advanced materials offer a variety of solutions that are based on the idea that “Materials are everywhere even in our body!”. Within these solutions, it is vital to consider the reuse of residues, recycling, and circularity to serve a Green Agenda and circularity and so, to proper shape our future.

In this regard, the role of advanced materials to contribute towards the future, as the driven force for the societal and economic transformations will be presented and discussed.

Invited and Oral Sessions

Hall 1

T6-I: Interplay between ferromagnetism, optical absorption and photocatalytic activity of semiconductors interfaced with a half-metal at nano-scale

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When a ferro (ferri) magnet of the half-metal type is interfaced with a semiconductor, at nanoscale, there is a charge transfer across the interface which involves only spin polarized states coming from or going to the Fermi level (FL) of the half-metal. If the FL of the half-metal is positioned above the semiconductor (SC) conduction band minimum (CBM) the spin polarized electrons will tunnel into the semiconductor at the CBM. Following the charge/spin transfer from the half-metal FL at CBM, several new properties will occur in the SC. First the SC becomes magnetically ordered via a double exchange process between single occupied anion vacancies and mediated by the common polarized electronic states tunneling through the interface (RKKY mechanism). The ferromagnetically ordered vacancies are oriented antiparallel with respect to the polarization source. Secondly, the presence of the neighbor

ferromagnet will determine a small but important Zeeman splitting of the initially spin-degenerate valence band states. Thirdly, band to band transitions through the absorption of photons with lower energy than that of the band gap are now possible. This is the specific case of cobalt ferrite as a partially inverted spinel interfaced into a core-shell structure with TiO_2 (doped and undoped with Tb). Here the lifetime of the photoexcited electrons in the conduction band increases due to their coupling with magnetically ordered interface transferred states. Also, the trapping of electrons into multiplet states of Tb^{3+} reduces the recombination rate. The photocatalytic efficiency of the magnetically ordered titania increases with respect to bare TiO_2 . The reactive oxygen species produced at the solid-liquid interface of TiO_2 were identified by Electron Spin Resonance coupled with spin-trapping technique. The results were correlated to the presence of the magnetic order inside the titania.

Acknowledgments The authors express appreciation to the Romanian Ministry of Research, Innovation and Digitization for the financial support through Project ELI-NP-17_2020 and JINR project 04-4-1142-2021/2025.

T6-I: Magnetic properties of $(\text{Zn};\text{Ni}(\text{Co}))\text{Fe}_2\text{O}_4/\text{SiO}_2$ nanocomposites

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We report on the magnetic properties of the nanocomposites (NCs) $(\text{Zn};\text{Ni}(\text{Co}))\text{Fe}_2\text{O}_4/\text{SiO}_2$ obtained by various preparation routes. Saturation magnetization (MS), remanent magnetization (MR), squareness (S), coercivity (HC), magnetic moment per formula unit (nB) and anisotropy constant (K) are very important parameters for a magnetic material to be used in technical and medical applications. The magnetic properties of these nanocomposite systems can be controlled by the chemical composition, the mean size distribution, the shapes, and structure of the nanoparticles and by the nature of the matrix in which they are embedded. The shape of the hysteresis loop revealed the dependence of superparamagnetic behavior on the structural properties. The replacement of magnetic Co^{2+} with zero magnetic moment Zn^{2+} in Co-ferrites induces a gradual reduction of magnetocrystalline anisotropy and the decrease of magnetic coercivity. The magnetic properties are strongly affected by the sample composition and cation distribution within the ferrite structure. The Ni-rich nanocomposites presented superparamagnetic behavior, while the Ni-poor nanocomposites ferromagnetic behavior. Both (MS), and (HC) increase with the degree of crystallinity, crystallite size and annealing temperature. The coercive field behaves differently for different heat treatment temperatures, increasing for 800 °C and decreasing for 1200 °C with increasing Mn content. The NCs with high Mn content heat treated at 1200 °C show superparamagnetic behavior, while those with low Mn content display ferrimagnetic behavior.

T6-O: Hydrogen-Mediated CVD Epitaxy of Graphene on SiC: Implications for Microelectronic Applications

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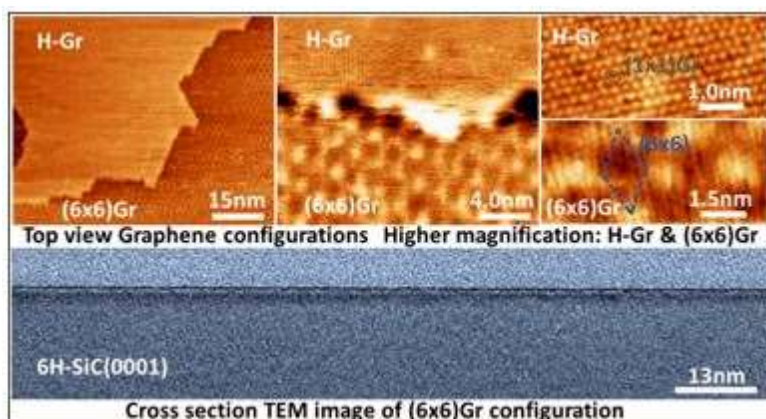
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Despite the large body of literature reporting on the growth of graphene (Gr) on 6H-SiC(0001) by CVD [1-3], some important issues have not yet been solved, and full-wafer-scale epitaxy of Gr remains challenging, limiting applications in microelectronics. With this study, we highlight the generic mechanism which produces the coexistence of two different atomic configurations of Gr: Gr on hydrogen (H-Gr) and Gr on buffer layer ((6 × 6) Gr), whose repartition and proportion can be controlled at will by changing the experimental conditions: from full coverage of H-Gr to full coverage of (6x6)Gr passing through a combination of alternating terraces covered either by H-Gr or by (6x6)-Gr [4]. We also demonstrated, for the first time, that graphene nucleates on purely hydrogenated SiC. Then, the desorption of H-atoms starting from step edges or defects leads to the formation of (6x6) Gr domains when hydrogen flow is below a critical value. Using the robust and generic X-ray photoelectron spectroscopy (XPS) analysis, we realistically quantify the proportions of H-Gr and (6 × 6) Gr

domains of a Gr film synthesized under any experimental conditions.



STM images showing the interface between H-Gr and (6x6)Gr domains existing on the same surface layer and their atomic structures. Large scale TEM image showing the continuity and homogeneity of (6x6)Gr configuration.

From these results, we can deduce that the H-assisted CVD growth of Gr developed here is a unique method to grow fully free-standing H-Gr in contrast to the method consisting of H-intercalation below (6×6) Gr epitaxial layer. Further description will be given in the presentation. These results are of crucial importance for future applications of Gr/SiC(0001) in nano- and microelectronics and in particular for field-effect transistors. We achieve thus a precise identification of new Gr surface structures which provide the groundwork for the use of Gr as an optimal template layer for Van der Waals homo- and heteroepitaxy for optoelectronic applications. In a last part, the

two different mechanisms of growth of Silicon on each accurately monitored Gr surface are reported.

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T6-O: Insights into electron transport in a ferroelectric tunnel junction

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The ferroelectric tunnel junction (FTJ) comprising of a thin ferroelectric film sandwiched between metallic electrodes is a quantum tunneling device for a wide range of applications like memories or solar cell[1]. FTJ is a voltage controlled device: the orientation of ferroelectric polarization can be switched by an external field. Due to incomplete screening and the asymmetry of electrodes, the depolarization field is nonzero and the potential profile is different for the two ferroelectric polarization states. Thus there is a switching of resistance, also known as the tunneling electroresistance (TER) effect. In principles, ab initio methods can provide a realistic picture of the FTJ physics in terms of structural, electronic, and transport properties [2]. However, for electron transport a semi-empirical approach is a useful tool to study FTJs and their TER effect [3]. In the present contribution we adopt a mixed approach. We will carry out first ab-initio calculations [4], in order to obtain many

of physical properties that are needed in the electron transport simulations, The electron transport calculations are performed with a numerical scheme similar to [3].

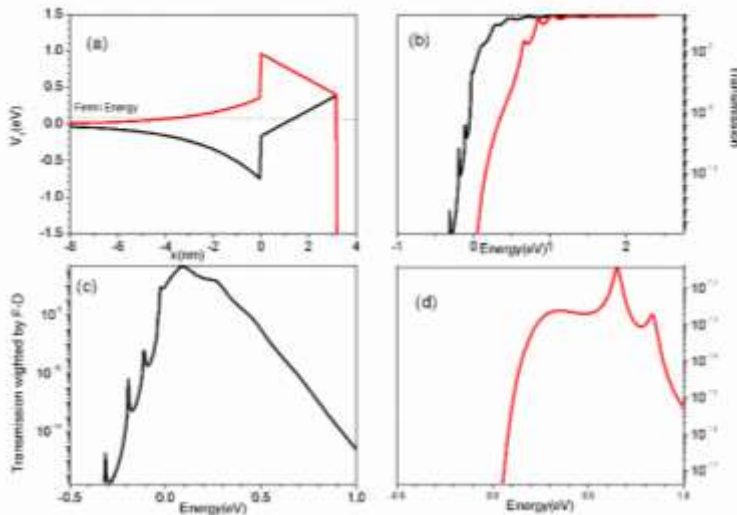


Fig.

1. A semiconductor/ferroelectric/ metal tunnel junction with positive (red) and negative (black) P: (a) its energy profile, (b) its transmission; and (c) and (d) the Fermi-Dirac weighted transmission.

The numerical scheme based is on the non-equilibrium Green's function and allows providing detailed information about the tunneling process. We show the case when the FTJ has a semiconductor as one of the electrodes (M1)-the left electrode in Fig. 1(a). It is a Nb doped SrTiO_3 [5]. The ferroelectric barrier is a 3.2 nm thick BaTiO_3 and the 2nd electrode is Pt. To simulate the doping a large Thomas-Fermi screening is adopted (2.5 nm). The polarization P is positive when it is from M2 to M1. In Fig. 1a are depicted potential profiles for positive/negative P . The graphs show a huge difference in electroresistance between

the two states of P, which is easily seen not only in the transmission(Fig.1b), but also in Fermi-Dirac weighted transmission, which gives the energy resolved current(Fig.1c,d). T is 300K. When P is negative a quantum well (QW) is developed on semiconductor side. This QW accommodates some quasi levels seen from the three peaks in transmission, for energies below 0 eV. It is shown also the thermionic part of the current.

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T6-O: Single crystal oxide nanoparticles synthesis using microwaves vaporization of metallic wires

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Single crystal oxide nanoparticles were synthesized using microwaves vaporization of metallic wires in air. An 800 W microwave generator was coupled through an antenna to a cylindrical wave guide cavity. The single-mode guide was constructed in accordance with TM011 propagation mode (transverse magnetic mode), which ensures that the electric

field of the microwaves is focalized on the symmetrical axis of the cylindrical cavity at around 6 cm away from the magnetron antenna. In that nodal position we placed on a ceramic plate, which is transparent to microwaves, the metallic wires of 5 cm length and less than 0.5 mm diameter. The wires were exposed for 10 s to the generated microwave field, resulting in their heating, vaporization and finally a plasma plume formation (see Fig. 1).

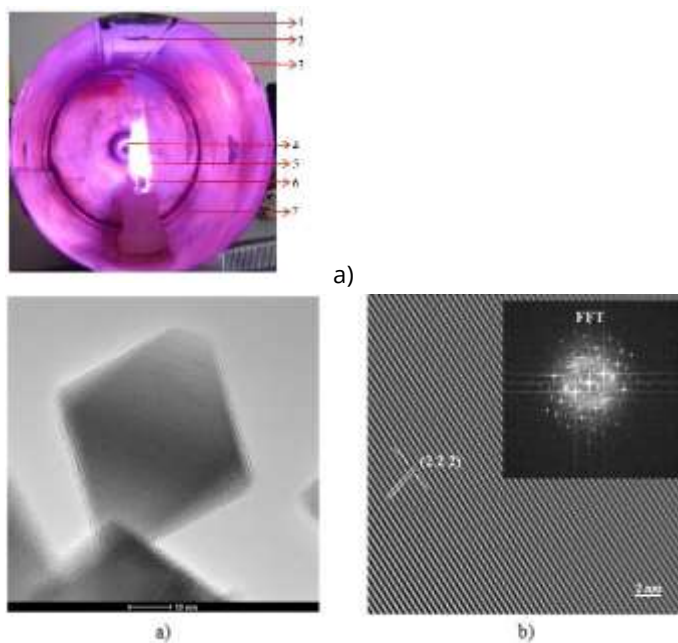


Figure 1. Image of the plasma formed when a metallic In wire was exposed to the microwave field in air: 1- thin film support, 2- deposited thin film, 3- cylindrical cavity, 4-magnetron antenna, 5-plasma, 6-ceramic support, 7-plastic support. Figure 2. HRTEM of In₂O₃ nanoparticles deposited on carbon film: detail (a) with Fast Fourier Transform (FFT) spectrum (b).

Optical emission spectroscopy investigations indicated that a high electronic temperature was reached in the plasma plume. The vaporized material was collected on a Si wafer placed opposite the wire, near the cavity wall.

Scanning electron microscopy investigations showed that the deposited material consisted of an agglomeration of nanoparticles. X-ray diffraction and transmission electron microscopy (TEM) investigations indicated that the nanoparticles were very crystalline, with random orientation. X-ray photoelectron spectroscopy analysis confirmed the formation of stoichiometric oxides. High resolution TEM investigations found that the nanostructures were single crystals, with faceted surfaces. This simple method could have many applications for metal nanocrystal oxides synthesis.

Figure 1. Image of the plasma formed when a metallic In wire was exposed to the microwave field in air: 1- thin film support, 2- deposited thin film, 3-cylindrical cavity, 4-magnetron antenna, 5-plasma, 6-ceramic support, 7-plastic support. a) b) Figure 2. HRTEM of In_2O_3 nanoparticles deposited on carbon film: detail (a) with Fast Fourier Transform (FFT) spectrum (b).

Online

T3-O: 1D-lantanides (La, Sm, Er) doped TiO₂ photocatalysts for degradation of organic pollutions

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In the last decades, the concept of environmental protection has become more and more complex due to environmental pollution having as source the rapid and continuous industrialization of the last century. Semiconductor photocatalysts have emerged as a good economical alternative for removing organic and inorganic environmental pollutants [1]. TiO₂ is one of the most important oxide semiconductors due to its optical, electrical and photochemical properties, low-cost and nontoxicity and having a high solar-energy conversion efficiency [2]. This work presents the preparation and characterization of lantanides (Ln=La, Sm, Er) doped TiO₂ unidimensional (1D) nanostructures with various composition ratios. The structure, morphology, optical and photocatalytic properties are investigated in detail, as a function of various Ln contents (0.025–1%). Effects of La-dopant content, calcination temperature, and different doses of photocatalysts on the

photodegradation efficiency were studied. The optimal level of La and the optimal temperature of calcination were 0.1% La and 600 °C, respectively. The photocatalytic degradation of methylene blue (91%, with a rate constant of $2.179 \times 10^{-2} \text{ min}^{-1}$) and ciprofloxacin (CIP) (99.5%, with a rate constant of $1.981 \times 10^{-2} \text{ min}^{-1}$) pollutants was highest on the (0.1%)La:TiO₂ annealed at 600°C, after 300 min irradiation under visible light. This photocatalyst displayed sustainable efficiency for CIP degradation up to five consecutive uses. Effects of Sm and Er dopant content on the photodegradation efficiency of the MB dye were investigated. The best catalyst sample of these series was formulated as TiO₂:Sm(0.1%) sintered at 600°C. This catalyst was employed for the intensification of the photocatalytic process (under visible light) by adding hydrogen peroxide to the system. Likewise, the chemometric approach was applied to optimize the process. Results revealed that for photo-degradation of the cationic organic pollutant, the rate constant was significantly improved ($k=3.496 \times 10^{-1} \text{ min}^{-1}$). In terms of the half-life of reaction, the process intensification and optimization led to dramatically drop of the half-life of reaction from 68 min to 2 min.

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T3-O: Study of the thermal degradation of vegetation from Oran's forest in Algeria

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Forest fires destroy the environmental balance and contribute to global warming. The recurrence of forest fires each year in pioneering countries such as the United States, Canada, Australia, Portugal and Greece demonstrates the current inability of operational and scientific staff to control this phenomenon. It is therefore necessary to characterize the flammability and combustion properties of forest plants. This characterization requires knowledge of the physical parameters involved in these processes. Indeed, a plant species may have different physical and chemical properties from one region to another. Simulation models of fire ignition and spread use parameters found in the literature.

The aim of this work is to characterize the dominant plant in Algeria, such as Aleppo pine needles, Eucalypt and olive leaves. Their parameters will be included in the simple physical model of inflammation of Koo et al [1]; among them, the most important is the heat capacity, which will allow adapting the elements of this simulation to concrete values.

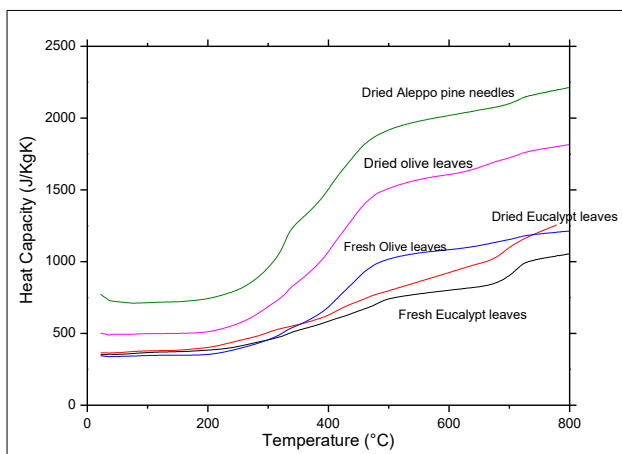


Fig.1. Temperature variation of the heat capacity

The purpose of this work is to study the thermal degradation process of different types of vegetation (by TGA analyses), to determine the phase transitions that occur and the variation of the specific heat along this process by varying the temperature (high temperature) under controlled atmosphere (by DSC analysis, using a reference sample [2]). Evaluation of combustion kinetics of vegetation at high temperature allows to determine the temperatures of degradation, the moisture absorbed by the material, and the quantity of organic compounds released [3].

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T3-O: Au/TiO₂/WO₃ composites' multiple applicability as photocatalysts and SERS materials

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In this present work, we synthesized Au/TiO₂/WO₃ ternary composite systems *via* the Turkevich *in situ* and impregnation preparation methods [1]. We investigated the morpho-structural and optical properties of the obtained products, their applicability as photocatalysts and SERS materials. We synthesized the composite systems from HAuCl₄ solution, commercial TiO₂ (Evonik Aeroxide P25), respectively from WO₃ synthesized from ammonium metatungstate hydrate (AMT) [2]. Concerning the synthesis of the ternary composite systems into 48.78 mL of distilled water, 750 mg of TiO₂ was added, and the suspension was stirred for 30 minutes. Afterward, 240 mg of WO₃-AMT was added, followed by another 30 minutes of stirring. We added 2 mL of 25.39 mM HAuCl₄ solution dropwise to the suspension, then heated to 90 °C. Upon reaching the needed temperature, 5.08 mL of (38.8 mM) sodium citrate dihydrate was added to the suspension and stirred for 60 minutes. Finally, the suspension was washed with distilled water and centrifuged; respectively, the samples were dried for 12 hours at 80 °C. We characterized the ternary composite systems' morpho-structural and optical properties by

employing Scanning electron microscopy, Transmission electron microscopy, Raman spectroscopy, and Diffuse reflectance spectroscopy. The photocatalytic applicability of the composite systems was evaluated by oxalic acid and phenol degradation under UV light irradiation. We assessed the SERS applicability of the composite systems by detecting crystal violet dye in small concentrations ($c = 10^{-7} - 10^{-8}$). Given the COVID-19 global pandemic, respectively, the increased administration of Coronavirus-related drugs (blood thinners, analgesics, and antipyretics) to infected patients, we have tried to remove the aqueous solutions Paracetamol and Aspartame drugs, with the ternary composite systems under visible light irradiation. In this present work, ternary $\text{Au/TiO}_2/\text{WO}_3$ composite systems with multiple applications as photocatalysts and SERS materials were prepared using the in situ and impregnation Turkevich method.

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T3-O: Investigation by electron spectromicroscopy of the interplay between surface chemistry and polarization landscape of ferroelectric surfaces

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The chemistry of ferroelectric surfaces is a fascinating subject nowadays, owing to the fact that charged surfaces feature a considerably increased chemical activity [1]. Additionally, near surface band bending act as sources of charge carriers for surface oxidation and reduction, natural or photo-induced [2]. In this work, we will study the stability of a 100 nm thin $\text{Pb}(\text{Zr,Ti})\text{O}_3$ (PZT) surface deposited on SrRuO_3 with a buffer electrode of SrTiO_3 under chemically active species (CO), X-rays and electrons fluxes by visualizing in real-time regions mapped by X-rays Photoemission Electron Microscope (XPEEM) and Near Edge Adsorption Spectroscopy-Photoemission Electron Microscopies (NEXAFS-PEEM). All these methods correlated with the Low Energy Microscopy (LEEM I-V), Secondary Electrons and Valence Bands maps informations afford us to discriminate between different polarization states and to understand the chemical states of the ferroelectric surface. In Fig. 1 reveal the dissociation of lead in red and orange areas. We observe the presence two different chemical states of lead: PbO and Pb^{4+} .

Experiments are performed at SMART beamline at BESSY II Synchrotron in Berlin. $\text{Pb}(\text{Zr,Ti})\text{O}_3(001)$ films are prepared by Pulsed Laser Deposition (PLD).

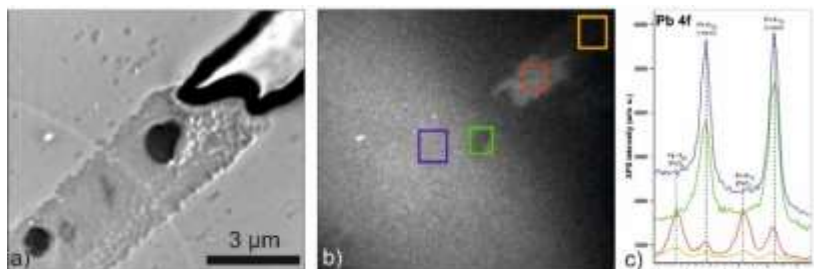


Fig. 1. Chemical states of the PZT(001) surface after annealing in oxygen atmosphere. a) Mirror Electron Microscopy (MEM) image of the area of interest, $E=2$ eV. b) XPEEM image of the same area obtained by energy filtering at binding energies corresponding to $\text{Pb}4f_{5/2}$ ($h\nu=215$ eV, $E=69-69.9$ eV). c) XPS spectra around Pb 4f peak taken from the regions marked by the colored boxes in b)

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T3-O: Synthesis and photocatalytic properties of titanium oxide nanotubes modified by heat treatment in glycerin

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Hydrogen is currently attracting a lot of attention as an environmentally friendly fuel. Its reserves are unlimited, and in the long term, they can replace traditional energy resources,

reducing their share in consumption. However, all existing industrial methods for producing hydrogen fuel (steam reforming of methane, water electrolysis, coal gasification) are environmentally unsafe due to the large amount of emissions into the environment. A more environmentally friendly way of producing hydrogen is the photoelectrochemical splitting of water into molecular hydrogen and oxygen under the influence of sunlight. Anodic titanium oxide (TNT) nanotubes, which have low cost, high chemical inertness, and developed surface area, are used as a suitable semiconductor material for a photocatalyst. However, the limiting factor of their large-scale application is the insufficient absorption of solar energy by TNT due to the large width of the forbidden zone. In this work, we propose an original method for modifying TNT using heat treatment in glycerin. The TNT arrays obtained in a fluorine-containing electrolyte were placed in glycerol heated to 200 °C for 60 minutes. The results of measuring the photocurrent showed that after the modification of the structure with glycerol, an increase in the photoactivity in the visible region of the spectrum is observed. Photocatalytic activity measurements show an increase in hydrogen generation by modified samples compared to unmodified ones. The results of this work can be used for further research in the field of increasing the photocatalytic efficiency of materials based on TNT.

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Nanostructured materials whose properties can be controlled in the fabrication process are very important in developing sensing functional devices. Regarding sensor fabrication, nanowires are the best candidates due to their high surface to volume ratio and ease of morphology control during their growth process. In order to have a fine control of key parameters such as chemical composition, diameter, length, doping, and electronic properties, we have used in this study electrochemical growth via template method. ZnO is a widely used semiconducting material in applications such as energy production, photocatalysis, light emitting devices, sensors or logic circuits due to its intrinsic physical properties, high occurrence/low cost and nontoxicity. When fabricated as nanowires, ZnO has very interesting properties especially in the area of field effect transistors. In order to optimize the fabrication process for adaptable sensing devices, we have studied the ZnO nanowires via scanning electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray diffraction and ultimately the electric properties were studied by contacting single nanowires to interdigitated electrodes (using electron beam lithography).

Tuesday, September 28, 2021

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- 08:00 **Invited and Oral Session**
HALL-1
- Poster Session**
- 08:00 Online
- 10:30 Coffee Break
- 11:00 **Invited and Oral Session**
HALL-1
- 11:00 **Invited and Oral Session**
Online
- 13:20 Lunch
- 15:00 **Plenary Session**
Online
- 18:00 **Coffee Break and Poster Session**
HALL 1
- 18:00 **Poster Session**
Online
- 20:30 Dinner

HALL 1**T5-I: Applications of terahertz time domain spectroscopy (THz-TDS)**

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Electromagnetic waves which lie between the microwave and infrared regions in the electromagnetic spectrum are known as terahertz (THz) waves and these waves cover the frequency range approximately from 100 GHz to 3 THz. Terahertz wave can be used to characterize wide variety of materials such as semiconductors, polymers, gases, biomolecules, amino acids, and pharmaceutical products, which makes it important for fundamental science, security, and medical applications. Measurement of such materials involves the use the terahertz time domain spectroscopy (THz-TDS), which is a technique that allow one to obtain both amplitude and phase of terahertz electric field. THz-TDS is widely used to measure material parameters such as refractive index and absorption coefficient of a sample using a single pulse of THz wave. Typical terahertz time domain spectroscopy in transmission geometry consists of femtosecond laser, terahertz emitter, detector and other electronics devices for terahertz wave measurement and visualization. A laser beam emitted by femtosecond fiber laser ($\lambda = 780\text{nm}$, repetition rate = 50 MHz, pulse width < 100 fs) is

divided into two equal halves using beam splitter. One half is used to pump the photoconductive antenna whereas other half, which travels through the optical delay line, is used to excite another photoconductive antenna used as a terahertz detector. The emitted terahertz wave is guided by off-axis parabolic mirrors and focused on the sample under investigation. Measurement of terahertz pulse transmitted through the sample enables us to obtain optical constants such as refractive index and absorption coefficient. In this presentation, I will explain the working principal of terahertz time domain spectroscopy in transmission mode for the characterization of different samples such as semiconductors and liquids. At the end of the presentation, I will show recent results from our lab related to in vivo measurement of human skin using attenuated total reflection terahertz time domain spectroscopy.

T5-O: Nanostructured metals as active layers for gas sensors

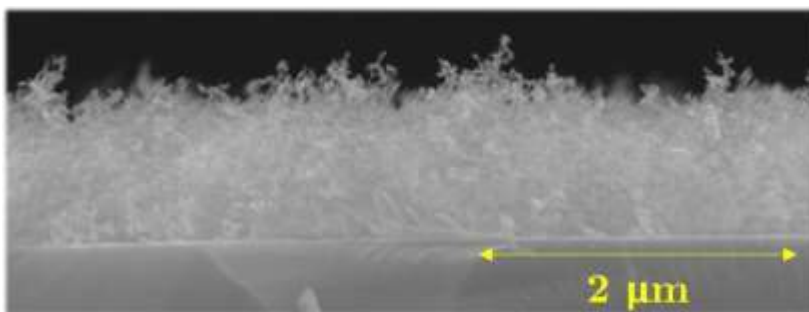
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Nanostructured and nanoporous metal layers (also called black metals) are highly promising materials for chemical gas sensor applications due to their fractal surface and high surface-to-

volume ratio. Nanostructured layers of black gold (BAu) and black silver (BAG) were deposited by thermal evaporation from a tungsten boat in an inert argon atmosphere at an elevated pressure of 100 Pa on quartz crystal microbalance (QCM) substrates and glass chemiresistor substrates with gold electrodes. The prepared layers were subsequently annealed to obtain different morphological structures with various sizes of pores. The layers were characterized by SEM, AFM, and UV-VIS spectroscopy. Prepared sensors were tested for several gas analytes, including NO₂. It was proven that highly nanoporous and nanostructured materials (such as metal blacks) provide more binding sites for analytes and hence increase the response of the QCM sensors. It was also observed that nanostructured metal layers exhibit electrical resistance higher than that of solid films and are therefore suitable as active layers for chemiresistors. Black gold and silver-based chemiresistors were tested for NO₂ detection with promising results.



SEM image of a cross section of a layer of black silver

T14-I: Nanocomposites and plasmonic nanostructures for broadband photodetectors and sensing applications

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Broadband photodetection, from UV to SWIR, is required in a large range of applications, such as imaging systems, optical metrology, bio-chemical sensing. optical metrology, bio-chemical sensing, colorimetric and multispectral imaging. The paper presents several types of solution processed photodetectors: hybrid device- PbS QDs/c-Si photodetector; PbS QDs photoconductor; ZnO NW- PbS:P3HT:PCBM ternary blend photodetectors; reduced graphene oxide (RGO):P3HT nanocomposite/n-type silicon photodetectors.

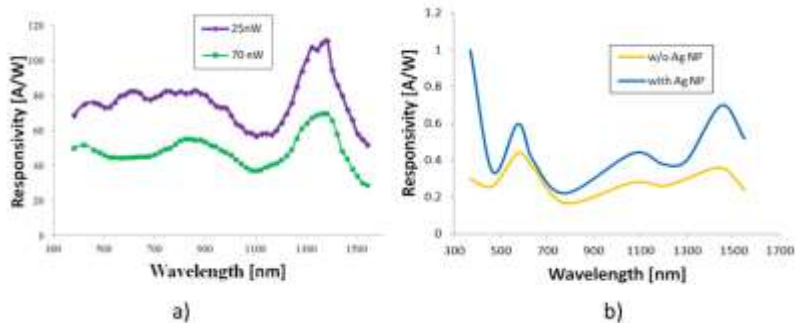


Fig. 1. Spectral responsivities for: a) hybrid photodetector PbS QDs/Si; b) ZnO NW- PbS:P3HT:PCBM ternary blend photodetector with and without Ag NPs.

We focused on solution processable materials based on quantum dots (QDs), nanowires and/or reduced graphene oxide (RGO) that can be synthesized in large quantities through solution routes and can easily be integrated with many substrates, including silicon and flexible foils. PbS QDs 5nm-

diameter have been used to obtain a good responsivity in SWIR and combination ZnO nanowires (NWs) -PbS QDs have been used to extend the spectral range both in UV and SWIR.

The P3HT:PCBM polymer blend was used to improve the absorption in the green range. Plasmonic nanostructures (Ag nanoparticles) have been also added to improve the photocurrent generation by light trapping and/or electromagnetic field local enhancement due to the excitation of localized surface plasmons (SPPs). Fig. 1 presents the spectral characteristics of two types of photodetectors. The obtained characteristics offer prospects use the device in multi-channel detection over a broad spectral range, from UV to SWIR.

Acknowledgments. The work was supported by the IMT core program MICRO-NANO-SIS PLUS, project 191601 funded by MCID under Grant 14N/2019, and by PN-III-P2-2.1-PED-2019-1300 MeatFlen and PN-III-P2-2.1-PED-2016-0307 TemptSys grants of MCDI- UEFISCDI.

T14-O: Nanostructured layers fabricated by Oblique-Angle Deposition (OAD) for optimizing optical performances in the extended visible range

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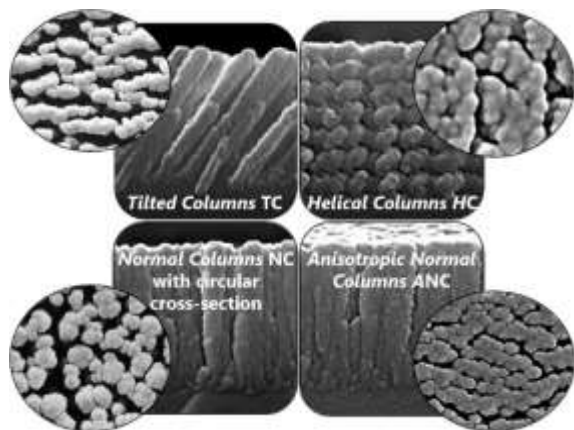
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Controlling the growth of nanostructured thin films is essential to optimize their physical, optical and chemical performances for future multifunctional systems. Oblique-Angle Deposition

(OAD) using electron beam evaporation, a bottom-up process, is a promising and original method for producing columnar and highly porous nanostructured materials used in many applications: photonics, solar cells, biomaterials, sensors. OAD can yield thin films with tailored refractive indexes promoted by the introduction of porosity by shadowing effects [1]. Additionally, the film morphology can be controlled by changing the substrate orientation during the deposition. The characterization of the resulting layers is complex due to their anisotropies and porosity gradients. Therefore, deep investigations are required.

In this work, the study of optical properties is mainly addressed.



SEM micrographs of OAD sculptured TiO₂ thin films fabricated.

The growth of sculptured nanostructures is controlled using unique means of elaboration. New morphologies have been fabricated (Fig.1) such as Normal Columns (NC) with circular cross-section, Helical Columns (HC), Anisotropic Normal Columns (ANC) and Tilted Columns (TC). These films were then characterized by Scanning Electron Microscopy (SEM), by spectrophotometry and by spectroscopic ellipsometry to understand the correlations between firstly elaboration

parameters and nanostructures and secondly between nanostructures and optical properties. The NC design is as efficient as the TC design in terms of optical performances and has undoubted advantages in optimizing existing antireflective coatings. Ongoing work related to the development of a new generation of antireflective functionality such as omnidirectionality [2] are also discussed.

[1] A. Barranco et al., *Progress in Materials Science* 76 (2016) 59–153.

[2] J. A. Dobrowolski et al., *Applied optics*, 41 16 (2002) 3075–3083.

T11-I: Formation, structure, and electrical properties of self-assembled monolayers on Ge as passivating and insulating layers

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Due to its high intrinsic mobility, germanium is emerging as a likely alternative material to replace silicon in the next generation of high-mobility and high-frequency field effect transistors. However, the preparation of an interfacial layer enabling to passivate and insulate Ge surface is still problematic. A promising approach consists in designing new self-assembled molecular monolayers (SAMs) [1] grafted on Ge exhibiting highly insulating and passivating properties as new high-K self-assembled nanodielectrics [2].

We have studied SAMs of model molecules such as alkylthiols and fluoro-alkylthiols, and of specially synthesized non-charged novel

push-pull chromophores bearing electron donor and acceptor groups, separated by a pi-conjugated bithiophene bridge which promotes electron transfer and a subsequent dipole formation [3]. Indeed, due to the alignment of the oriented dipoles promoted by the SAM deposition strategy, such push-pull chromophores have been shown to form highly polarizable insulating films in the literature [2]. We have adapted and developed the original Ge deoxidation/grafting technique in hydro-alcoholic solution [4] and shown that, compared to the usual deoxidizing acid treatment, it gives smoother surfaces and well-organized SAMs, which is proven by ellipsometry, wettability, and scanning probe microscopy analyses. The grafting of alkylthiols and fluoro-alkylthiols on Ge has been performed directly in a single step, whereas for the push-pull chromophores designed with a carboxylic anchoring group, we have achieved a two-step grafting with amide bonding on pre-assembled amine-terminated sticking layers. Among the latter, we have demonstrated aminothiophenol SAMs exhibit a better arrangement than cysteamine, with a smooth monolayer film suitable for grafting ordered push-pull SAMs on top. UV-Visible absorption spectroscopy of push-pull chromophores in solution was used to determine the concentration limit to avoid aggregation. X-ray photoelectron spectroscopy (XPS) and infrared spectroscopy (FTIR) analyses demonstrate the oxide removal from the Ge surface after the SAM formation.

Statistical electrical analyses revealed that with such push-pull SAMs, we have been able to decrease the current by a factor of 10^5 compared to Ge, and 10^4 compared to dodecane SAMs of similar thickness. Results have been analyzed by transition voltage spectroscopy [5], and successfully correlated with spectroscopic analyses of molecular levels, using inverse photoemission spectroscopy and XPS valence band determination for probing the unoccupied and occupied molecular orbitals respectively, as well as with DFT calculations, thus allowing to identify the highest occupied

molecular orbital as the level involved in the electronic transport through the push-pull SAM. Dipole formation has also been evidenced in the SAM.

- [1]. A. Ulman, *An Introduction to Ultrathin Organic Films*, Academic Press (Ed.), Boston (1991)
- [2]. A. Facchetti et al., *Adv. Mater.* 17 (2005) 1705; Y.G. Ha et al., *Chem. Mater.* 21 (2009) 1173
- [3]. V. Malytskyi et al., *Tetrahedron* 73 (2017) 5738
- [4]. J.N. Hohman et al., *Chem. Sci.* 2 (2011) 1334
- [5]. X. Lefevre et al., *J. Phys. Chem. C* 119 (2015) 5703

Poster Session

Online

T1-P: Solution processed reduced graphene oxide thin films on glass substrate for photodetection applications

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In this work we present the synthesis process of RGO and deposition on transparent glass substrate and the optical, electrical and morphology investigation of the prepared thin films. To evaluate the photoresponse were prepared metal-RGO heterostructures in two configuration, one with interdigitated coplanar electrodes (Cr/Au-15/200 nm) and another with vertically arranged metal electrodes. Reduced graphene oxide sheets are prepared starting from graphene oxide (GO) obtained by Hummers method. The graphene oxide was investigated before centrifugation as a neat material (GO)

including bi-, tri- and multilayers of un-exfoliated graphite oxide and after centrifugation a sample was taken from supernatant solution (GOs) and the solutions were further centrifuged at 2000 rpm for 2 minutes to remove unexfoliated multiple layers of graphite. RGO was obtained from supernatant GOs and further dried at 80°C temperature in hydrazine vapors atmosphere. In Fig. 1 are presented typical Raman spectra acquired on the samples containing RGO, GOs and GO and inset is shown decomposition and representation of RGO-D, G and D' Raman bands.

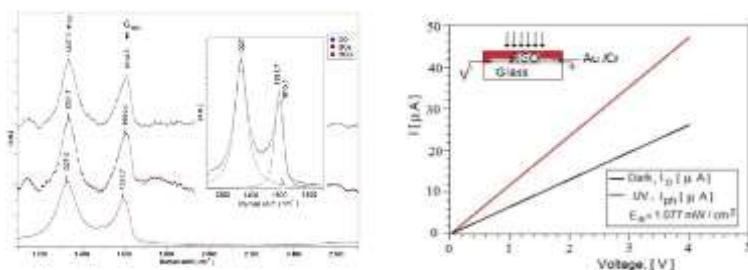


Fig.1 Typical Raman spectra acquired on GO, Fig.2 Photocurrent versus voltage under UV irradiance.

The quality of prepared RGO was investigated by analyzing Raman spectra both by classical method using intensity ratio, I_D/I_G and by introducing a new Raman - the difference between the positions of D' and G bands. Due to superposition of the G band (1582 - 1591 cm^{-1}) and D' band (lattice vacancies at $\sim 1615 - 1620 \text{ cm}^{-1}$ in graphene) in RGO gives rise to an apparent G band - G_{app} .. After processing Raman spectra collected on RGO samples we found that the difference is in the range (28.3 - 21,521,5 cm^{-1}), this range can be viewed as uniformity indicator for any RGO sample. Photocurrent versus applied voltage in coplanar configuration of the Au-RGO-Au electrodes under UV irradiance of $E_e = 1.077$

mW/cm² is presented in Fig. 2. The I-V characteristics recorded in dark, white light and the UV irradiation confirmed the photodetection properties of the metal-RGO heterostructures.

Acknowledgments. This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, PNCDI III project NANODEC - 427PED/2020.

[1] Mustaque A. Khan¹ · Karuna K. Nanda¹ · Saluru B. Krupanidhi, J Mater Sci: Mater Electron (2017) 28:14818–14826

[2] Abid, Poonam Sehwat, S. S. Islam, Prabhask Mishra & Shahab Ahmad, Scientific REPOrTS | (2018) 8:353

T1-P: Experimental setup for optical films Laser-Induced Damage Threshold measurements

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The advent of high-power laser systems (HPLS) (i.e., ELI-NP, 2 × 10 PW) has involved the development of large optical components with high optical qualities. One of the most important qualities that limits this development is the laser-induced damage threshold (LIDT). Any optical component must be tested before being inserted into a HPLS. We proposed an experimental system (see Figure 1) capable of determining in real time optical properties such as: (I) nonlinear coefficients

(nonlinear refractive index, nonlinear absorption coefficient [1]), (II) LIDT using a long working distance imaging system (LWDIS), (III) spectral broadening. The proposed experimental assembly has the following advantages: laser system based on Ti: Sapphire amplification (800 nm, 10 Hz) similar to HPLS, femtosecond pulse duration (60 fs), LIDT in transmission and reflection (dedicated to coated surfaces), 10 Hz, 1-on-1 or S-on-1 LIDT qualification methods and is completely automatized.

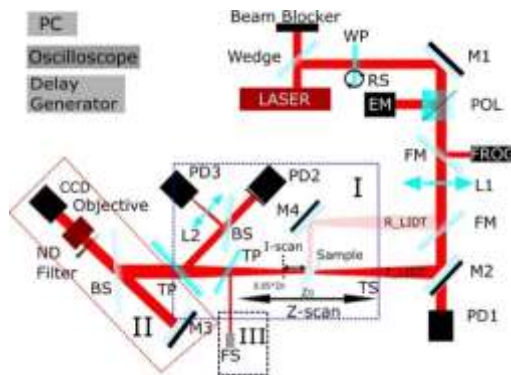


Fig.1. Experimental Setup

The qualification of the initial parameters (energy, duration, surface) and of the method was made according to ISO 21254 standards 1-4 [2]. Following the LIDT measurements, the fluence at which the material or coating was destroyed was determined. Such an example can be seen in Figure 1 (before and after the material was destroyed). In the present example, an HfO₂ thin film deposition on fused quartz substrate by the pulsed laser deposition technique was used. The results showed that this type of deposition can be safely used into HPLS at fluences greater than 300 mJ / cm².

Acknowledgements. This work was supported through IFA project ELI-RO 4/2020 LPTC.

[1] I. Dancus et al., Z-scan and I-scan methods for characterization of DNA optical nonlinearities, *Romanian Reports in Physics*, 65 (3) (2013) 966-978;

[2] ISO 21254-1-4, Lasers and laser related equipment.

T1-P: HfO₂/AlN multilayer devices and their functional characterization

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The ferroelectricity in hafnium-based materials was very recently discovered and boosted the development of nanoscale thin films for use in electronic technology. At the same time, AlN attracted the attention of scientific community due to its high thermal conductivity and chemical stability in harsh environments.

The use of these two materials together, as HfO₂/AlN multilayers, opens the window toward the intriguing negative capacitance (NC) effect and it's applicability in electronics.

The HfO₂ layers were obtained by ALD technique starting from tetrakis(ethylmethylamino)hafnium and H₂O precursors. The AlN insulator was deposited by sputtering a pure aluminum target in nitrogen reactive atmosphere.

The HfO₂/AlN multilayers were integrated in MIS and FET structures together with indium-gallium-zinc oxide as semiconductor. Their electrical output is discussed relatively to the single layer HfO₂ or AlN based devices.

T1-P: The effect of nickel concentration on electrical and mechanical properties of high-entropy -AlCoCeFeNi_x alloy and -(AlCoCrFeNi_x)N Nitride thin-film coatings synthesized by pulsed laser deposition

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The class, which serves today's most industrial needs, entitled High-Entropy Alloys (HEAs) is obtained from a minimum of 5 main elements in equiatomic or near equiatomic proportions ranging from 5% to 35%, being a multi-component material with single- or multi- close-packed cubic and hexagonal structures. This transition, from traditional to complex alloy systems, was initiated for research and properties enrichment purposes. Within this research, HEAs of three different nickel concentrations obtained by arc remelting from high purity raw materials were used as targets. We report the thin film coatings obtained based on single-phase Face-Central- or Body-Central-Cubic (FCC or BCC) structures of AlCoCrFeNi_x HEA, with x of 0.2, 1.2 and 2.0, which have been irradiated by means of laser ablation, and deposited on Si, Ti and glass substrates. For enhanced mechanical properties in industrial applications, however, High-Entropy Nitrides (HENs) coatings proved to be an even more promising candidate [1]. Therefore, we report the

deposition parameters of the obtained nitrides thin film coatings as well.

The first investigations implying Grazing Incidence X-ray Diffraction (GIXRD) and X-Ray Reflectivity (XRR) revealed the thin film coatings' physical properties. The element concentration of coatings determines the electrical properties, measured by Four Point Probe (4PP), and, moreover, it is shown that, as the Ni and N₂ contents increases, the conductivity decreases. Therefore, by assessing how the Ni [2] and N₂ contents affects conductivity, we report the microstructure of concerned coatings as well, recorded by means of Scanning Electron Microscope (SEM), Fig. 1.

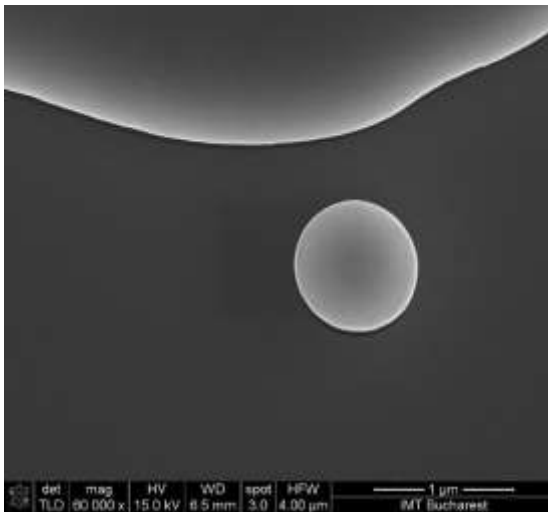


Fig.1 Microstructure of AlCoCrFeNi_{2.0} or HEA10 thin film coating deposited in N₂ environment

Further, the atomic % of elements, which were obtained with the aid of Energy Dispersive X-ray Spectroscopy (EDX), and, for comparison reasons with X-Ray Photoelectron Spectroscopy (XPS) are presented. Besides, the mechanical properties of the

synthesized HEAs and HENs were studied using indentation and the hardness parameters were recorded. The low friction coefficient establishes which coatings are suited for the requirements of hard- or soft- coatings for extreme environments.

[1] Synthesis and characterization of super-hard AlCrTiVZr high-entropy alloy nitride films deposited by HiPIMS.

[2] Effects of nickel content on the microstructure, microhardness and corrosion behavior of high-entropy AlCoCrFeNi.

T1-P: The effect of thickness on the properties of gold and silver thin films

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In the present work, we studied noble metals (i.e., Ag and Au) thin films with thickness values in the range 2 – 9 nm and prepared by rfMS technique onto glass substrates.

A comparative analysis was conducted by measuring the thickness of the corresponding oxide thin films using scanning electron microscopy (SEM), interferential microscopy (WLI) and stylus profilometry methods. Surface profiles of the investigated samples indicated that size of the crystalline grains increased with thickness. Thinner films were less crystalline and had smaller crystalline grains. AFM images showed that our samples have a grain-like surface morphology. The surface roughness played an important role in nucleation and growth processes of those thin films. The crystallites orientation,

granulation and columnar growth were more evident in the Au samples.

The thickness effect on the compositional properties of these thin films were discussed based on XPS results. The scans show the presence of Au 4f5 and Au 4f7 in the gold nanostructures and of Ag 3d3 and Ag 3d5 in the silver ones, respectively.

The Ag and Au thin films have a strong orientation after the main planes perpendicular to the substrate. The intensities and positions of (111) peaks in the XRD patterns were strongly dependent on the thickness. Thus, increasing the thickness of the thin film greatly improved the crystallinity of the film. These thin layers present interest for advanced technologies in terms of basic research and new potential research for the next generation of spatial microsatellites.

T1-P: Compositional and optical properties by simulating the theoretical models of Ag/SiO₂/Si thin films grown with radio frequency magnetron sputtering deposition

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The small size of nanostructured layers is essential in applications of the miniaturized optical systems. We analyzed the silver thin films deposited onto the SiO₂/Si surface with thickness values in the range 4 – 10 nm. The deposition rate of radio frequency magnetron sputtering technique had a significant effect on the formation of uniform and continuous Ag film on the surface of SiO₂/Si. We obtained a multilayer of

Ag/SiO₂/Si, which has excellent qualities when the silver has 5 nm thickness, with plasmonic properties useful for obtaining structures with negative refractive index. Silicon dioxide has 300 nm thickness and high-performance dielectric properties, which improve the properties of metamaterial structures.

The deposition conditions were optimized and led to layers with a good morphology of surface, consisting of nanoparticles with dimensions between 7 nm to 15 nm and a surface roughness between 0.2 nm to 1.3 nm. The surface topography of samples was analyzed using scanning electron microscopy. The analyzed XPS general scans showed the presence of Ag 3d₃ and Ag 3d₅ in the silver nanostructures, which increased in quantity with the increasing predefined thickness of the film. The XRD diffractograms indicated that the Ag samples are crystalline. In the case of Ag samples, the orientation was clearly after the main planes perpendicular to the substrate for the (111) planes. It also proved, the increasing thickness of the Ag thin film on the surface of SiO₂/Si improved the crystallinity of the film. Good structural properties of the Ag/SiO₂ multilayer were highlighted by the crystallographic quality using XRD analysis and a high spectral transmission in the visible and infrared range.

The low resistivity of Ag/SiO₂ multilayer improves the electrical properties of the films, which is useful in metamaterial structures. The obtained films have a controlled morphology suitable in future applications of structures with metamaterials.

T1-P: Preparation of CuInSe₂ Thin Films by Spin-coating Method Using the Nanoparticles of CuInSe₂

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Copper indium diselenide, CuInSe₂ (CIS), and copper indium gallium diselenide, Cu(In,Ga)Se₂ (CIGS), attracts much attention as a promising compound of the next generation high conversion efficiency thin film solar cells, because it has a large absorption coefficient of the order of 10^5 cm^{-1} , which is approximately two orders of magnitude larger than that of crystal or amorphous silicon. These thin film solar cells have achieved conversion efficiencies exceeding 20% [1]. They also have excellent radiation and cosmic ray tolerance and are suitable as solar cells in space applications. Recently, a supply shortage in the market for metallurgical-grade silicon has been identified, and it is hoped that such solar cells will become low-cost thin-film replacements for the Si solar cells that comprise approximately 90% of current market share. Therefore, it is important that CIS and CIGS thin films are prepared by the wet process (spin-coating, electro-deposition, screen printing *etc.*) using the solutions in order to prepare large area solar cells applicable for the mass-production with low-cost [2, 3]. For one thing of them, it has the wet process using the solutions of nanoparticles of CIS or CIGS, and many studies related to them have been reported [4]. The aims of the present research were to prepare CIS thin films on quartz substrates by the spin-

coating method using the nanoparticles of CIS, and to establish the preparation parameters.

The nanoparticles of CIS used as a starting material to prepare the solution for spin-coating had an average particle diameter of 75-125 nm. The solvent was used a mixed solvent of ethanol and α -terpineol in a volume ratio of 1:1. The solution was prepared by mixing the nanoparticles of CIS and the solvent. The concentration of the nanoparticles of CIS per total weight was 10 wt%. The quartz substrates were spin-coated with the mixed solution at 2000 rpm for 15 s to obtain precursor films. The spin-coated films were dried at 100 °C for 10 min, and subsequently the sintering of the spin-coated films was carried out at 550 °C for various sintering time in nitrogen gas (N_2) atmosphere by rapid thermal processing (RTP) using an infrared (IR) lamp heating system to obtain CIS thin films.

Figure 1 shows SEM images of (a) surface morphology and (b) cross-section of CIS thin film prepared in the atmosphere of N_2 including Se vapor using nanoparticles of CIS. Surface morphology was shown a relatively small aggregate of particles and obtained CIS thin films including a lot of microcrystalline CIS. The cross-section showed an almost homogeneously crystallized layer with a vertical thickness of 4.0 nm and can be seen consisting of large grains that was grown up in the horizontally. We concluded that the improvement of crystallinity of CIS thin films was relatively effective for the sintering time and the sintering in Se vapor.

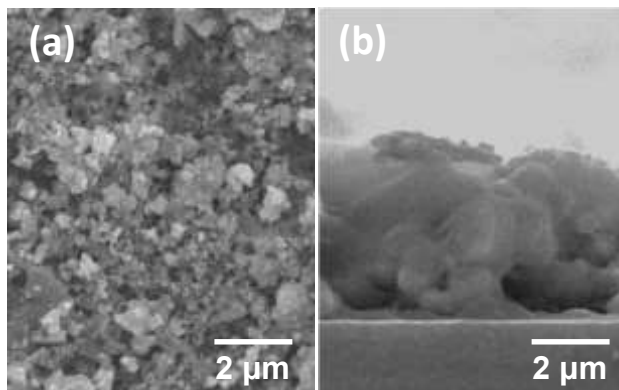


Fig.1. SEM images of: a) surface morphology, b) cross-section of CIS films

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T1-P: Effect for Annealing in O₂ atmosphere of Fe₂O₃ Thin Films Prepared by the Spin-Coating Method.

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In nowadays, silicon (Si) based solar cells are occupied approximately 90% of the global market share of solar cells. However, the Si raw material has a serious problem that is the rise in prices and the supply shortage. Iron oxide (Fe₂O₃) is attracted much attention as a promising material for the light absorption layer of the next generation high conversion efficiency thin film solar cells, because it has a large absorption

coefficient of the order of 10^5 cm^{-1} . This material is present inexhaustibly on the earth. In addition, harm to the human body is less, and is a material which is kind to the environment. In this work, Fe_2O_3 thin films were prepared by the Coating Thermal Decomposition method using an iron naphthenate as a raw material. The prepared Fe_2O_3 thin films were investigated the optimum manufacturing conditions by evaluating the surface state, luminous transmittance, and crystalline.

The manufacturing procedure for Fe_2O_3 thin films on quartz substrates by the coating thermal decomposition method is as follows. In the first, the Fe naphthenates solution were spin-coated on quartz substrates to obtain precursor films with smooth surface. Next, the spin-coated films were heat-treated "Pyrolysis process" at 450°C for 15 min using an IR lamp in air. These procedures were repeated five times. Finally, the pyrolysis of film was carried out at 800°C for 30 min in air in order to crystallize Fe_2O_3 thin films.

Fe_2O_3 thin films were prepared at sintering temperature of 800°C for sintering time of 30 min in the air. From the XRD pattern, the spectrum of Fe_2O_3 thin film showed the diffraction peaks peculiar for the intrinsic hematite structure ($\alpha\text{-Fe}_2\text{O}_3$). From the spectrum of optical transmittance, Fe_2O_3 thin films prepared at the same condition was shown the optical absorption edge in the vicinity of 590 nm (2.1 eV). On the other hand, Fe_2O_3 thin films prepared in O_2 atmosphere was good crystallinity compared with that of prepared in air. It considered that the oxygen vacancies in Fe_2O_3 thin films was promoted the introduction of oxygen atoms due to preparation in the O_2 atmosphere.

T4-P: Depicting bound vortex-antivortex pairs in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ superconductor

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We use magnetic scanning transmission x-ray microscopy at low temperatures to image individual vortex-antivortex (V-AV) pairs in a high temperature superconductor ($\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$) [1]. As sensor layer it is utilized a thin ferrimagnetic lamella, which is polarized by the local stray field induced by an individual superconducting flux line. With this method, we are able to visualize and analyze individual V-AV pairs at temperature much under the transition temperature with great spatial resolution and high contrast. We observed the V-AV pairs to nucleate spontaneously at the domain wall of the ferrimagnetic layer. Our results are the first identification of a bound and stable V-AV pair and demonstrate the potential of the x-ray method to access the properties of vortices in high temperature superconducting thin films and heterostructures.

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T10-P: Effect of aging temperature on corrosion susceptibility, local-mechanical properties and microstructure evolution of 2507 super-duplex stainless steel

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The effect of annealing temperature ranging from 650°C-1200°C for 1hour on the pitting corrosion resistance of 2507 super-duplex stainless evaluated in 3.5% NaCl solution has been investigated. SEM analysis revealed that the degradation of corrosion resistance were strongly influenced by sigma phase precipitation Increasing the annealing temperature to 850°C resulted in the decrease of the pitting resistance whereas the best corrosion behavior is obtained after 1200°C aging treatment. Microstructure examination revealed a preferential corrosion that occurred primary in ferrite and Cr-depletion zones i.,e. secondary austenite which exhibited the lowest pitting resistance equivalent. Furthermore, it is found that the initiation of pitting corrosion took place around the newly σ phase and Cr₂N nitride that nucleated in δ/γ and δ/δ boundaries.

Aging temperature, 2507 SDSS; microstructure; corrosion performance.

T10-P: Interfacial evolution of WC-Co/AISI 304L diffusion bonded joint obtained by flash SPS technique

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In this work, WC-Co cermet was successfully joined to AISI 304L stainless steel using flash spark plasma sintering (FSPS) technique under a constant load of 5 MPa with ultra-rapid holding times (Fig.1). The results revealed that increasing the holding time to 12s resulted in massive interfacial deformations accompanied with an important diffusion activity of Co, Ni and Fe. The residual stresses measurements conduced in the WC phase showed compressive stresses in the joints obtained using less than 8s holding time. Whilst, tensile stresses are found in the joints using 10s and 12s holding time.

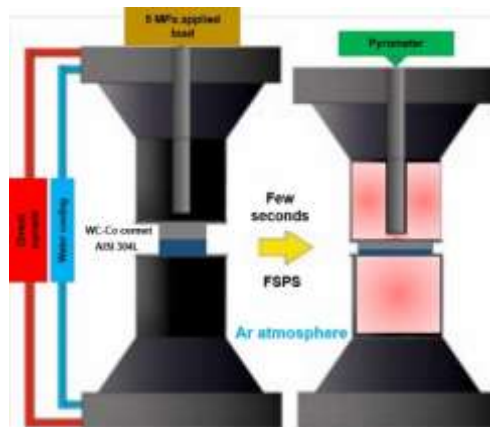


Fig. 1. Welding processes using SPS technique

The difference in stress results is attributed, on the hand to the, inter-diffusion phenomenon that accentuate with increasing holding time and, on the other hand, to the brittleness of the WC-Co cermet resulting in the cracks appearance along the WC-Co/AISI 304L interface Toughness measurement of WC-Co cermet at the vicinity of the bonding interface using Vickers indentation fracture (VIF) method showed that the mechanical properties of the bonded joints are deteriorated and their brittleness is increased with increasing the holding time, although, the significant inter-diffusion phenomenon that occurred between the WC-Co cermet and the 304L steel constituents.

Conclusion The key issues of this work are summarized as follows: - Flash SPS process is believed to be an effective technique to perform an acceptable WC-Co/steel joints with an appropriate holding time considering the other parameters. - At the joint interface, the inter-diffusion of Ni, Fe and W elements is activated by the plastic deformation which became more prominent with holding time. - Increasing the bonding time results in the brittleness of the WC-Co cermet that causes the premature failure of the weld joint. - Compressive residual stresses are obtained whatever the bonding time, which decrease due to the cracks appearance and the structure relaxation near the interface.

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T10-P: Effect of ageing on microstructure and mechanical properties of LDX 2101 Lean duplex stainless steel

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In the present paper, the precipitation behavior in Lean Duplex Stainless Steel (LDX) 2101 was investigated. The precipitates were detected by XRD and confirmed to be mainly Cr₂N, together with some M₂₃C₆ particles. After solution treatment at 1050°C, the Lean duplex alloy presents a typical ferritic-austenitic duplex structure. Isothermal ageing treatments were carried out at 720°C for different holding times. The precipitates at δ/γ interface preferentially nucleated and grew into the ferrite phase, when increasing isothermal ageing times (Fig.1).

The ferrite/austenite (δ/γ) interface migrated from the precipitate particles into δ phase, leaving the precipitates behind along the original interfaces, which could increase the size of the secondary austenite phase and decrease the hardness values of both austenite and ferrite. During aging, a relationship between microstructure and a corrosion resistance was revealed which was associated to the formation of chromium- and molybdenum depleted zones around the precipitates.

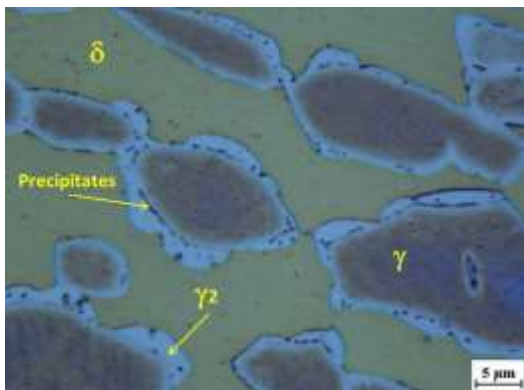


Fig.1. Optical micrograph of lean duplex aged at 720°C during 72 hours

T10-P: Electrochemical behaviour of pulsed and alternate TIG AA6061-T6/ ER5183/ AA5086-H32 dissimilar weldments in an ASTM G69 solution

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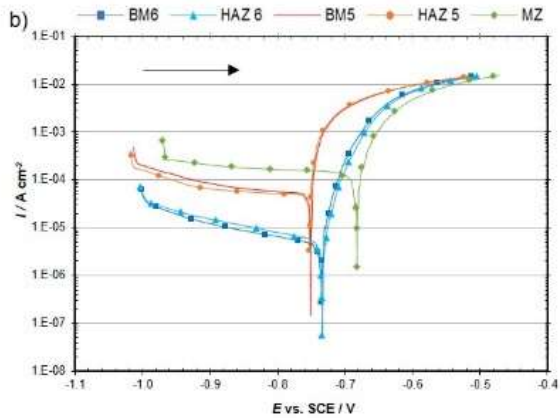
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Two dissimilar weldments of AA6061-T6 with AA5086-H32 aluminium alloys using ER5183 as the filler metal were manufactured using pulsed and alternate current Tungsten Inert Gas (TIG) welding.

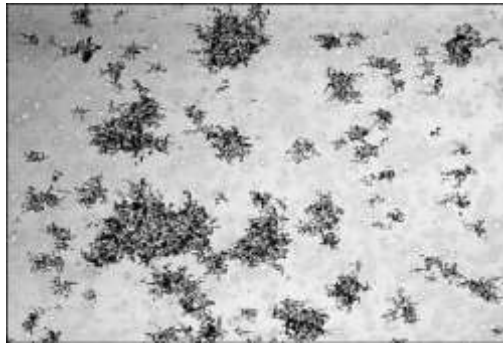
The electrochemical behaviour of each part of the welds was evaluated in a NaCl + H₂O₂ solution (ASTM G69). To obtain reliable data, the setup parameters for the electrochemical tests were experimentally assessed.

Then, the open circuit potentials and corrosion current densities of the base metals and respective heat affected zones were recorded. The results suggest that the welding

parameters have very little influence on the corrosion behaviour of these dissimilar weldments.



a)



b)

Fig.1. a) Aluminium Alloys, TIG Welding; b) Electrochemical reaction; pitting corrosion

T3-P: Modification of the surface of the cathode material NMC 622 using $\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$

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Lithium-ion batteries (LIBs) are widely used in consumer electronics, mobile phones, personal computers, as well as in hybrid and electric vehicles [1]. Cathode material NMC 622 is one of the most promising for use in high-capacity LIBs. However, NMC-type materials suffer from an interphase reaction between the cathode material and the liquid electrolyte, which reduces the specific power and impairs the cyclicity of the cathode material.

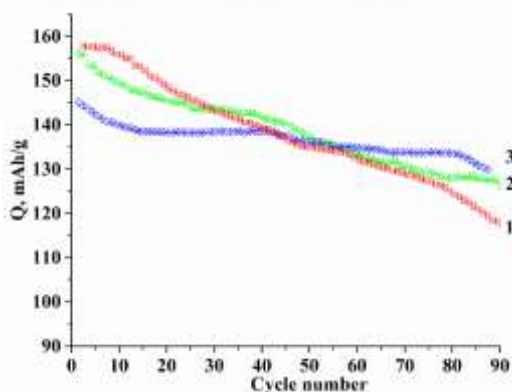


Fig.1. Change in the specific capacity of the pristine NMC and cathode materials with a protective layer of LATP: 1 – without LATP protective layer; 2 – LATP protective layer applied mechanically; 3 – LATP protective layer applied by a sol-gel method.

To prevent interfacial side reactions, composite systems have been proposed in which a shell of chemically stable (in contact with the electrolyte) and electrochemically inert materials (such as FePO_4 , Al_2O_3 , AlPO_4 etc.) is applied to the particles of the NMC cathode material [2]. In [3] the authors showed that solid electrolytes, in particular lithium-aluminum-titanium phosphate with NASICON structure, can be used to create a protective shell on the particles of cathode materials. In this work, the influence of the method of creating a protective layer on the surface of the NMC622 cathode material on its electrochemical characteristics was investigated for the first time.

It was found that the creation of a protective layer of nanoparticles of solid electrolyte LATP using two methods (mechanical application and sol-gel method) It was found that the creation of a protective layer of nanoparticles of solid electrolyte LATP using two methods (mechanical application and sol-gel method) can significantly increase the stability of the capacitive characteristics of the cathode material during a long-term charge-discharge cycling as shown at Fig.1. However, applying the LATP protective layer to the particles of the NMC 622 cathode material by the sol-gel method is a more promising technology, as it reduces the capacity drop during a long-term cycling by almost 2.5 times compared to the cathode material without a protective layer. In addition, the application of a protective layer of LATP using the sol-gel method can significantly increase the capacity of the cathode material at high current density. The results obtained provide a basis for a systematic study of the effect of the deposition of a protective

LATP layer by the sol-gel method on the electrochemical characteristics of other layered cathode materials with the NMC type structure.

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T3-P: Deposition and characterisation of off-stoichiometric Cu-Cr-O thin films on flexible substrates

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Transparent conductive oxides (TCOs) are a class of materials that exhibit both high electrical conductivity and optical transparency, which are typically mutually exclusive material properties. The lack of a p-type TCO with properties comparable to their n-type counterpart is still restricting the fabrication of a fully transparent p-n junction, a technological breakthrough in the field of transparent electronics. In addition, the investigation of p-type TCOs grown on flexible substrates is scarce. Our group reported previously off-stoichiometric copper-chromium delafossite ($\text{Cu}_{0.66}\text{Cr}_{1.33}\text{O}_2$) with long Cu vacancy chains as source of high p-type electrical conductivity and adequate optical transparency. In this work we report the properties of Cu-Cr-O successfully grown by chemical vapour deposition on two different flexible substrates – Schott® and Upilex®. Thermoelectric measurements confirmed the p-type conduction and demonstrated high carrier concentration

typical for a degenerate semiconductor. This might allow the application of fully transparent active devices on flexible substrates.

T4-P: Laminated magneto-electric composites for sensing applications

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The fabrication of highly efficient integrated magnetostrictive sensors, actuators and transducers requires the availability of magnetoelastic materials with high magnetostriction and low saturation fields in different shapes, depending on the final application. In this work, we investigated the sensing properties of new laminated magneto-electric composites obtained by superposing magnetostrictive melt-spun ribbons on piezoelectric supports (PZT) in order to obtain high magneto-electric coupling coefficient and high sensitivity to magnetic field. Polycrystalline Fe-Ga (consisting of a mixture of disordered bcc and DO3 phases) and amorphous Fe-Si-B melt-spun ribbons with thicknesses of about 27 μm and different widths have been prepared by rapid quenching. The ribbons are magnetically soft, with a preponderant in-plane long axis anisotropy. The magnetostriction coefficients (λ_s) of the ribbons were determined by the small angle magnetization rotation (SAMR) method from the tensile stress dependence of anisotropy field [1,2]. The obtained values of λ_s are about 110

ppm for Fe-Ga ribbons and, respectively, about 30 ppm for Fe-Si-B ribbons. The laminated composites were obtained by gluing the ribbons (different numbers and disposed in different configurations) on the PZT support. The sensing properties of the laminated magneto-electric composites were studied in dynamic mode by measuring the electrical voltage given by PZT when the system is subjected to the action of a variable magnetic field AC and in the presence of a continuous magnetic DC bias field [3]. The sensing properties of the laminated composites strongly dependent on the width, the number, the configuration, and the intrinsic mechanical stresses induced in the superposed ribbons. These aspects will be discussed in detail in the paper.

Aknowledgements. Financial support by the NUCLEU Program (PN 19 28 01 01) is gratefully acknowledged.

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T4-P: Improvement of magnetic properties for Mo doped Ce-Fe-B ribbons

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Ce-Fe-B magnetic materials have developed in recent years as an alternative capable of filling the energy gap between hard ferrites and Nd-Fe-B magnets [1-2]. However, the magnetic properties of Ce-Fe-B materials are much inferior as compared to those of Nd-Fe-B materials [3], therefore efforts are being

made to improve them. A successful solution to improve the magnetic properties are addition and substitution of a small but critical concentration of elements [4]. In this respect, we report here the effect of Mo as substitution for Fe, on the magnetic properties and microstructure of $\text{Ce}_{14}(\text{Fe}_{78-x}\text{Mo}_x\text{Co}_2)\text{B}_6$ melt-spun ribbons prepared by rapid solidification ($x = 0, 0.5, 0.75, 1, 1.25$ at.%). The alloy ingots were prepared by arc-melting from the constituent elements (purity better than 99.9%), followed by induction melting in order to obtain better uniformity. $\text{Ce}-(\text{FeCoMo})-\text{B}$ ribbons were obtained by ejecting the melt from a quartz tube onto the surface of a rotating copper wheel, at different velocities, under argon atmosphere. The ribbons were then annealed in vacuum, for different periods of time, at temperatures between 630 °C and 700 °C in order to obtain the 2:14: phase. We have managed to achieve a coercivity near 3 kOe at RT in $\text{Ce}_{14}(\text{Fe}_{77}\text{Mo}_1\text{Co}_2)\text{B}_6$ melt-spun ribbons, annealed at 650 °C for 20 minutes, while the saturation magnetization was 91 emu/g. The microstructure of the annealed $\text{Ce}_{14}(\text{Fe}_{77}\text{Mo}_1\text{Co}_2)\text{B}_6$ melt-spun ribbon revealed a fine and uniform grains structure, with an average size of about 40 nm. Acknowledgements This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P2-2.1-PED-2019-2054, within PNCDI III

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T5-P: Metalloporphyrins as chemical sensors for food freshness assessment

200

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Three metalloporphyrins (Zn, Co and Mn) have been tested as electrochemical sensors for the detection of histamine in fresh meat products. TCA (trichloroacetic acid) has been used as mediator for the reaction. In our electrochemical setting, we used a screen printed electrode with two working electrodes onto which different metalloporphyrins have been immobilized. This type of electrode allows the detection of a low quantity of histamine. We obtained good results for the electrochemical detection of histamine with Co- and Mn-porphyrins, while Zn porphyrin is better suited for detection of histamine by absorbance (optoelectronic method). Keywords: histamine detection, porphyrin functionalization, double working electrode, electrochemistry.

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T5-P: Oxidized carbon nanohorns/PVP/KCl- based ternary nanohybrid as sensitive layer for resistive humidity monitoring

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Considering the importance of relative humidity (RH) control and monitoring in various industrial, commercial and domestic applications, the RH sensors development benefitted from a significant research interest in the last decades. Graphene oxide and oxidized carbon nanohorns (CNHox) have been mentioned recently, besides the traditional materials used in RH resistive sensors [1]. This paper reports the RH sensing response of resistive RH sensor incorporating a sensitive film based on a ternary nanohybrid CNHox - PVP (polyvinylpyrrolidone) - KCl at the masic ratio of 7:2:1. The developed RH sensing structure consists of a Si substrate, a SiO₂ layer, and two interdigitated (IDT) electrodes. The drop casting method was used to deposit a stable dispersion of CNHox - PVP - KCl in isopropanol onto the IDT structure, and its RH sensing capability was investigated.

Thus, the new sensor was exposed to different RH levels, and, while applying a current between the two interdigitated electrodes, the resulted voltage was measured.

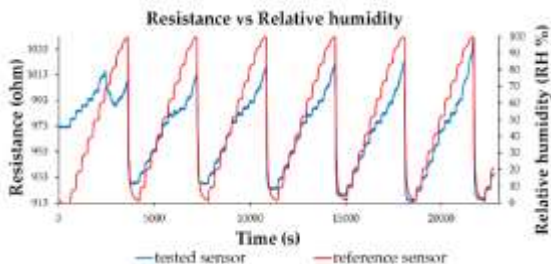


Fig. 1. Resistance vs. relative humidity, for a number of 6 cycles (RH: 0% - 100% - 0%)

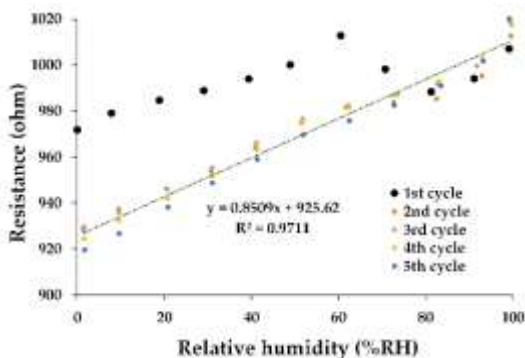


Fig. 2. Resistance of the tested sensor vs. relative humidity

The corresponding resistance was calculated, and correlated with RH values, as well as with the response times. In Fig.1 the first functioning cycle stands out, as the exposure to nitrogen with relative humidity over 60% produces a drop of the measured resistance of the tested sensor. Starting with the second operating cycle, the sensor's response is repeatable and with a very good linearity, as seen in Fig.1 and Fig. 2. Two types of sensing mechanisms are identified and discussed.

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T9-P: Towards the development of functional neurosurgery electrode probes with directional carbonic macro-contacts - Unconventional technologies and materials

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We report on our ongoing work towards enhancing the recording and stimulation capabilities of the acute investigation electrodes used during functional neurosurgery for deep brain stimulation (DBS) implantation procedures. Our proposed intraoperative probe is designed to enable multichannel directional stimulation and macro-recording, based on circumferentially segmented contacts, in correspondence with the technological trends applied also in the construction of implantable DBS leads. In addition, the patterned distal

contacts are based on a graphitic composite, thereby exploiting both its large water window, and capacitive charge transfer.



Schematic of the acute electrode probe with directional carbonic macro-contacts

The electrode will be finally linked to a miniaturized wireless headstage for improved user experience, recording quality and patient comfort. The architecture of the new probe (Fig. 1) reveals the main specificity of this development: the need to precisely pattern high aspect-ratio conductive channels, and carbonic contacts, on and around a non-planar substrate (small-radius cylinder). We have explored solving these unconventional tasks by various technologies and we will present the most promising.

Invited and Oral Sessions

HALL 1

T7-I: Digital manufacturing of functional materials and electronic devices: a step forward to green electronics

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How can we fabricate environmentally friendly functional materials and electronic devices?

Recent strategy in the electronics sector is to ascertain the ways to make more environmentally friendly functional materials and electronic devices. With this framework, the Inkjet printing



technology (IJP) is with no doubt one of the most promising technologies to reduce the harmful radiation/ heat generation but also achieve reductions of the waste material and the manufacturing cost.

IJP is capable of revolutionizing the whole system of manufacturing of both functional material and electronic devices including material selection, design and fabrication steps and device configuration and architecture opening a new field - Green electronics.

In the context of the manufacture of functional materials and electronic devices, ink jet printing offers a number of benefits, some of which are presented in Fig. 1.

This talk will encompass the potential of inkjet printing technology as an innovative manufacturing pathway for functional materials and electronic devices such as two

terminal memory devices, as a reliable alternative to traditional manufacturing protocols.

Fig. 1. The image shows the main features of inkjet printing

T3-I: Perovskite solar cells and future prospects for energy conversion-storage devices

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Development of perovskite solar cells (PSCs) based on $\text{CH}_3\text{NH}_3\text{PbI}_3$ has attracted worldwide attention from both academia and industries and became one of the best choices for solar energy applications. All materials in PSCs are abundant, and the solution processing used to make them is potentially cheap. In just ten years, power conversion efficiency (PCEs) jumped from 3.8% to 25.5% exceeding the record efficiency of CIGS solar cell and approaching that of mono Si-solar cells. Despite extensive research in cells efficiencies the intermittency constitutes one major limitation for substituting conventional fossil fuels energy resources. Integration of the solar cells with energy storage devices (batteries or supercapacitors (SCs)) into single device may solve this problem because of the concomitant electricity storage.¹ In this context, we aim to connect PSCs with SCs via a common carbon electrode (Fig. 1). To obtain activated carbon (AC) for both devices, biomass materials can be used as a renewable source which can help us to reduce the non-sustainable use of fossil carbon deposit.

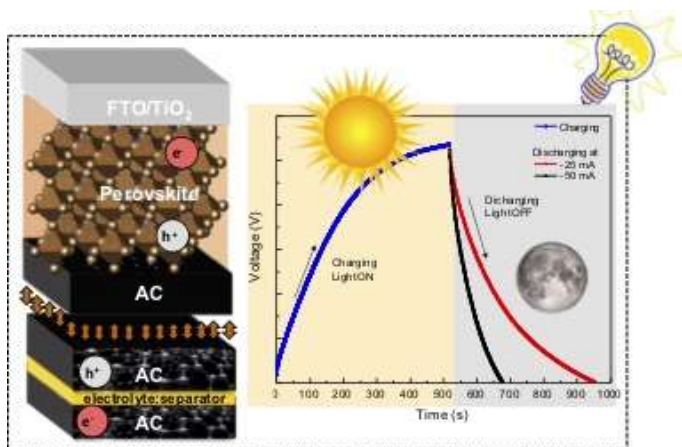


Fig. 1. Integrated device: carbon-PSC/carbon-SC.

T3-I: Porous oxides with bimodal pore size as catalysts support for CO₂ transformation in useful compounds

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The porous materials with bimodal pore size represent a class of catalytic supports containing pores of two distinct dimensions. These materials show promising properties for the adsorption and activation of the reagents through two mechanisms: the smaller pores should increase the surface area and enhance the metal dispersion, while the larger pores should facilitate the transport of reactants and products to/from the catalytic active sites. In this presentation two classes of bimodal pore catalysts were prepared, characterized and tested in CO₂ transformation in methane and synthesis

gas. First class of materials used silica as catalyst support while the second class were deposited on alumina. Nickel was the active metal for all catalysts. To increase the surface basicity lanthanum and cerium oxide were also deposited on support. The alumina supported catalysts were prepared by refluxed co-precipitation while the silica based one by means of a solvothermal method followed by successive calcination and Ni impregnation. All samples were characterized by XRD to establish the crystallinity of the support and the size of Ni crystallites, N₂ adsorption-desorption to calculate the surface area using BET method and the porosity using Dollimore-Heal model, TEM-EDX to analyze the size and dispersion of nickel nanoparticles, Thermoprogrammed Reduction (TPR) to estimate the strength of the metal-support interaction, Thermoprogrammed desorption of hydrogen and carbon dioxide (H₂-TPD and CO₂-TPD) to estimate the type and strength of catalytic active sites. All materials presented bimodal porous structure with larger pores size at least double compared to smaller pores for one specific sample. The large pores have the dimensions between 17 and 36 nm while the small ones between 8 and 16 nm. The best catalytic activity for both processes was obtained for lanthana containing catalysts due to the cumulative effects of: (i) improved capacity to activate both hydrogen and carbon dioxide, (ii) the combined effect of Ni nanoparticles stabilization inside the small sized mesopores, and the facilitated access of reagents to active centers due to the large mesopores. The used catalysts preserved the bimodal pore structure.

T3-O: Reflectometry studies of planar interfaces for lithium power sources

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Rapid development of electrical transport, robotic technologies, minimization and functional improvement of portable electronic devices demands accumulators with high capacities. Nowadays, the highest specific capacity is reached in lithium-ion batteries of the intercalating type. The prospects are foreseen for the batteries with metal electrodes, especially lithium anodes. However, the processes on electrochemical interfaces with liquid electrolytes are not fully understood, which slows the progress in this area. This concerns the controllable formation of solid electrolyte interphase (SEI), as well as the inhomogeneous lithium deposition on metal electrodes, which both affect performances and safety operation of such kind of batteries. The given work reports about the applications of X-ray (XRR) and neutron (NR) reflectometry to study planar interfaces related to lithium power sources. At the first stage, XRR is used for controlling and optimizing substrates for neutron experiments. It is well suited

for determining the initial comparatively simple structures with thin (thickness ~50 nm) metal electrodes deposited (magnetron sputtering) on crystalline silicon. More complicated heterostructures including multilayers with regulated mean scattering length density in quasihomogeneous approximation are also tested in the frame of the general task of optimizing NR experiment [1,2]. This problem appears, since the changes of the working electrochemical interfaces are small, and certain steps are to be done to enhance relative reflectivity changes during interface evolution. The application of NR makes it possible to investigate at a new level the influence on the interface evolution of the initial characteristics of anode surfaces, environmental parameters, electrolyte composition, overvoltage, current density. For this purpose, electrochemical cells for simultaneous monitoring of voltage/current at the interface under study together with the organization of the neutron beam passing through the interface, followed by the detection and analysis of the scattering are designed [3]. The results of the adaptation of the NR experiment to study the structure of electrochemical interfaces are summarized.

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T3-O: MIL-53 – alumina composites as alternative in the methanation of CO₂

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The exceptional physico-chemical properties of metal-organic frameworks (MOFs), such as high surface area, tunable porous structure, compositional and structural versatility, as well as tailorability, have made these compounds very attractive candidates for catalytic applications [1,2].

In the case of CO₂ methanation, MOFs can play an important role since activation of both reactants can be achieved due to (1) the enhanced dispersion of active metal particles inside the ordered porous structure of the MOF, leading to improved activation of H₂, and (2) due to the gas sorption and storage capacity which is beneficial in respect to the activation of CO₂. Despite these extraordinary advantages, MOFs' usually low mechanical and thermal stability, as a consequence of their large porosity and low density, are important disadvantages for heterogeneous catalytic applications. Therefore, unless an efficient way to shape MOFs is found which preserves the unique properties, their catalytic application in the methanation of CO₂ will not reach an endpoint.

The aim of this work is to report the synthesis of MIL-53-alumina composites with enhanced mechanical stability as compared to MIL-53 alone, and their potential use in the

methanation of CO₂. Our strategy was to use alumina pellets, known for their high thermal and mechanical stability, and to cover them uniformly with MIL-53. In order to do so, a solvothermal procedure using only water as solvent was used, besides the reactants (terephthalic acid and Cr or Al precursors to give MIL-53 with either Cr or Al as metallic nodes). The complete characterization of the MIL-53-alumina composites by nitrogen adsorption-desorption isotherms (BET method), powder X-ray diffraction (XRD), thermogravimetric analysis (TGA), or electron microscopy revealed that these composites retain the properties of both MIL-53 and alumina. MIL-53-alumina based catalysts used in the methanation of CO₂ revealed improved performances as compared to the homologues alumina or MIL-53 based catalysts. Acknowledgement: This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2019-1447, within PNCDI III.

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T3-O: Bias-Field Effects in Spatially Heterogenous Ferroelectric Thin Films

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Ferroelectric thin films attract a particular interest due to their potential applications in photovoltaics, spintronics, high-density data storage, ultrafast recording, microactuators, or broadband microwave phase shifters. For most of these applications, highly crystalline thin films are needed. Granular $\text{Bi}_2\text{FeCrO}_6$ (BFCO) double perovskite thin films were grown by pulsed laser deposition on Nb-doped SrTiO_3 (001) (Nb:STO). Because of the mismatch of 0.77%, the films are therefore strained on the substrate which has impact on the local properties of BFCO [1]. In this sense, the ferroelectric properties are explored using piezoresponce force microscopy (PFM). The sample exhibits an asymmetric polarization hysteresis loop with respect to the external bias voltage which indicates the presence of a bias field at the interface. This effect corroborates with a preferential ferroelectric polarization direction as the loops becomes wider with a significant displacement of one of the switching fields when the sample is poled in the opposite direction with respect to the preferential polarization direction. A partial recovery of the asymmetry of the hysteresis loops is obtained when the sample is poled back in its preferential polarization direction. This demonstrates a mutual influence between the polarization and the interface bias field. The findings can be of relevance for all strained ferroelectric thin-film materials obtained by epitaxial growth on atomically flat substrates.

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Online

T10-I: Molecular dynamics of species belonging to nematic liquid crystals of alkyl benzoate type and to their composites with oxide nanopowders

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Our group has worked on the behavior of molecules confined to restricted geometries [1]. However, the molecular mobility of the liquid crystals (LCs) from the series of 4-pentyl phenyl 4-alkyl benzoates (5PnB, n=number of carbon atoms in the alkyl chain) in bulk or in composites with aerosil A380 is much less studied than that of the related series of cyanophenyl alkyl benzoate (CPnB) (e.g. [2]). In fact, the molecules of 5PnB are more flexible than those of the members with the same alkyl part in the cyanobiphenyl (nCB) or CPnB series and can form trans and cis isomers. Molecular mobility of the species derived from 4-pentyl phenyl 4-propyl benzoate molecules (5P3B) was investigated by broadband dielectric spectroscopy (BDS) in a large temperature range. High silica density (> 7 g aerosil/1 g of the LC) was selected to gain information on the interaction between a thin LC layer and the surface of aerosil nanoparticles on which it is adsorbed. Infrared spectroscopy and

thermogravimetry measurements sustain the BDS investigations, Bulk 5P3B is monotropic and shows the expected phase transitions. For the composites one relaxation process is observed at frequencies much lower than those for the bulk; it was assigned to the dynamics of 5P3B molecules in the surface layer. The temperature dependence of the relaxation rates and of the dielectric strength shows a crossover behavior with two distinguished regimes. At higher temperatures the data obey the Vogel–Fulcher–Tammann law, whereas an Arrhenius law is observed at lower temperature, in a close similarity to the behavior of a constrained dynamic glass transition. We intended to receive effective dielectric properties of our heterogeneous nanostructured materials, using Maxwell Garnet and also Bruggeman theory [3] but this goal needs more studies. Acknowledgements. This work was funded by Ministry of Research, Innovation and Digitization [Project PN19-030101 under 21N Core Program]. Aerosil A380 was a gift from Degussa-Huels and the LC comes from Nemoptic by courtesy of D. Stoenescu. The authors appreciate the valuable contribution of Stefan Frunza, recently deceased.

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T10-I: Raman spectroscopy as a versatile tool for multifunctional oxides characterization

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Several examples of applications of Raman spectroscopy for the characterization of multiferroic materials will be presented. A method based on the Raman tensor formalism was employed for the assignment of the BiFeO_3 Raman modes of pure as well as mixed character/symmetries. Using this assignment, it is shown that Raman spectroscopy is a powerful tool for the investigation of ferroelastic domain formation in multiferroic materials, being able to probe the tilt of the domain walls in the case of macrodomains. [1] On the other hand, Raman spectroscopy was also used for understanding temperature induced structural phase transitions in BiCrO_3 , and in the mixed BiFeO_3 - BiCrO_3 systems (thin films and polycrystalline materials). The simultaneous presence of Fe and Cr in these systems results in a strong electron-phonon interaction. The latter has been investigated employing different excitation wavelengths.

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T10-O: Effect of varying Cu content on structural and surface properties of Co&Cu co-doped ZnO thin films

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Co&Cu co-doped ZnO thin films with a fixed Co content of 1 at % and various Cu contents (1, 3, and 5 at %) are grown by sol-gel dip coating method on microscope glass substrates. The deposition voltage and temperature for 10 cycles of dipping are chosen as 24 V and 500 °C, respectively. The structural properties of ZnO thin films are analysed by X-ray diffraction (XRD) method. The lattice parameters of the films are determined from XRD patterns. The crystallite size, strain and stress are obtained for all films by applying Williamson-Hall (W-H) [1] method. Surface properties are investigated using atomic force microscope (AFM) and scanning electron microscope (SEM) measurements. The elemental composition of the films is confirmed by the energy dispersive X-ray (EDX) analysis.

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T1-I: Flexible thin films based on Te-SnO₂ nanocomposites and their gas sensing properties

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Printed electronics becomes very attractive due to the ability of using sustainable, compostable and recyclable materials including biobased plastics and paper in the elaboration of different flexible thin-film sensors, transistors and systems [1]. In this talk I will present information related to development of flexible sensors based on printable Te-SnO₂ nanocomposites for the detection of toxic and pollutant gases at room temperature. A brief review of fabrication, physical properties and application of both elemental tellurium and tin oxide in technology of the chemical sensors is reported and discussed in context of the development of the novel nanocomposites based on these very different semiconducting materials. Being synthesized these nanocomposites appeared to be suitable for the application in printed electronics for fabrication of flexible gas sensors, enabling low-cost fabrication through computer aided designs.

The fabrication route of Te-SnO₂ nanocomposites consists of solvothermal recrystallization of pure (99.999 %) crystalline tellurium in acids. The composition and structure of synthesized nanocomposites were investigated by energy-dispersive X-ray spectroscopy (EDX) and XRD. Flexible thin films based on Te-SnO₂ nanocomposites have been fabricated and their surface morphology studied via scanning electron

microscopy (SEM). The films were cut and used as active elements in developed devices for detection of toxic gases in ambience at room temperature.

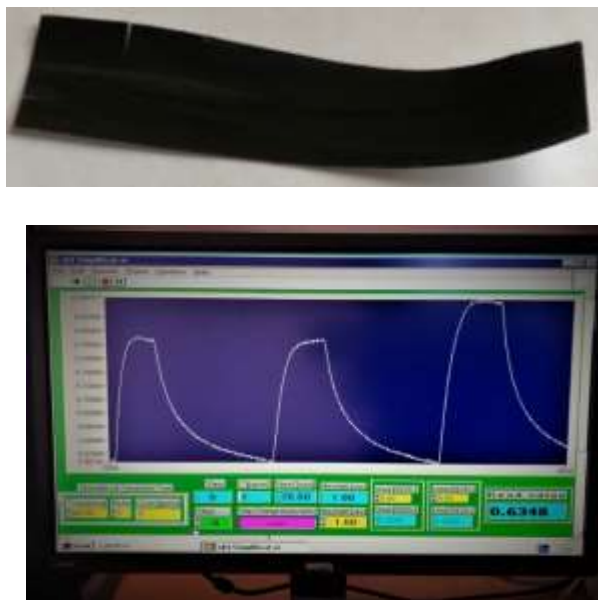


Fig.1.The image shows the view of a flexible thin film based on Te-SnO₂ nanocomposites and its dynamic response to rectangular pulses of 1.0 ppm in ambience.

Fig.1 shows the image of a fabricated flexible thin film based on Te-SnO₂ nanocomposites and dynamic response of such a film under exposure to rectangular pulses of a very toxic gas (NO₂) of a low (0,1ppm) concentration in ambient air. Gas sensing characterization of such films was realized dependent on concentration of different gases, temperature and humidity of the ambience. The sensing mechanism is proposed and discussed.

T1-O: Investigation of some conjugated push-pull naphthalene-based imines for potential use in optoelectronic applications

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The field of organic electronics based on vinylenic organic compounds has been intensively investigated in the last years. A feasible alternative to vinylenic-based materials is represented by imine (or azomethine) π -conjugated compounds.^{1,2} These derivatives possess many advantageous features, like thermal and chemical stability, semiconducting properties, complexation ability etc., some attributes which recommend them for use in different applications. The optoelectronic properties combined with the simple synthesis and easy purification make imine derivatives good candidates for use as thin films in electronic devices with application prevalently in the field of optoelectronics.³ By embedding two types of units, one with electron-withdrawing and another with electron donor characteristics in imine conjugated molecules can lead to new push-pull systems. This approach for structural modification of imine derivatives may endow them with high degree of conjugation, enhanced electron transport and excellent optoelectronic properties. In this study we report the synthesis and characterization of some imine oligomers containing naphthalene units. The ¹H-NMR and FTIR

spectroscopies studies were employed in order to confirm their envisaged structure. The thermogravimetric analysis was used to evaluate the thermal stability which proved to be very high. The ability of molecular packing in solid state was found to be affected by the solvent used for deposition, with direct consequence on film morphology. The positions of the UV-Vis absorption maxima were also found to be affected by the solvent, particularly by its polarity. The cyclic voltammetry investigations were carried out to survey the imine electrochemical behavior, with emphasis on electronic transport characteristics. The band gap energy values were estimated by electrochemical method and compared with those obtained by the Tauc analysis. The results of this study evidenced that the synthesized push-pull imine can be used as active layers for optoelectronic applications. Acknowledgements: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-PD-2019-1026, within PNCDI III

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T1-O: Substrate effect for efficiency control of Al-CuOx multilayer reactive microsystems

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Currently, progress in micro- and nanoelectronics is associated not only with a decrease in the topological dimensions of logical elements, but also with an increase in the level of integration. The development of technologies and methods for creating three-dimensional assemblies, systems on a chip or on crystal, micro- and nanoelectromechanical systems, will allow for the transition to advanced technologies and systems. Development of methods for joining groups of components, incl. thermosensitive, using local heat sources based on multilayer thermite materials is one of the promising universal approaches to solving the problem of creating a reliable joint of various surfaces. However, in order to create effective local heat sources with specified characteristics, it is necessary to solve the most important scientific problem - the determination and prediction of the energy properties of multilayer thermite materials, taking into account their chemical composition, size effects, properties of the surfaces and substrates being joined. From a practical point of view, it is necessary to solve the problems associated with the development of methods for the formation of integrated energetic microsystems - energetic materials with specified characteristics formed in certain areas. Traditionally, thermal management refers to the design of microelectronic devices and devices with the aim of maximizing heat dissipation and minimizing local heating. Within the framework of this work, the opposite problem is solved, associated with the understanding and precise control of heat

dissipation in the process of a self-propagating reaction in multilayer thermite Al-CuOx materials on the surface of various substrates. In addition, an experimental study of the influence of heat accumulators or barriers at the "energy material - substrate" interface on the propagation velocity of the wave combustion front has been carried out.

T1-O: Optical and photosensitive properties of flexible n(p)–InSe/In2O3 heterojunctions

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InSe is a typical representative of group III–VI layered materials, with room temperature band gaps of about 1.3 eV (direct) and 1.26 eV (indirect). Single crystalline lamellae, obtained by splitting InSe crystals perpendicularly to the C6 axis, are comprised of elementary Se-In-In-Se packings, bound by van der Waals forces, with closed valence bonds at surface. Due to mentioned characteristics and low surface-state density, InSe is considered among the first 5 most promising materials for photovoltaic, water splitting and transistor technology applications [1]. In this work, optical, photoluminescence and photosensitivity characteristics of micrometer-sized flexible (n– and p–InSe)/In2O3 heterojunctions, obtained by heat treatment in water vapour

and oxygen enriched atmosphere of single crystalline Cd- and Sn-doped (0.1–3.0 at. %) InSe lamellae, have been investigated. Thin films of In-Cd alloy were used as electrodes. The absorption edge of In₂O₃:Sn and In₂O₃:Cd structures on InSe substrate was studied by means of ultraviolet reflectance spectroscopy. The direct band gap of native oxide, determined from its reflection band edge, is equal to 3.45 eV and ~ 3.52 eV for In₂O₃ layer on InSe:Cd and InSe:Sn substrates, respectively, for doping concentrations 0.1- 0.5 at.

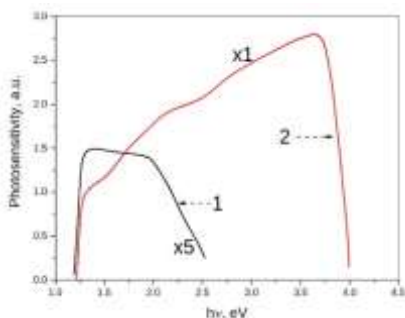


Fig. 1. Relative spectral photosensitivity of n⁺-In₂O₃/n-InSe:Sn (curve 1) and n-In₂O₃/p-InSe:Cd (curve 2) structures.

In₂O₃ exhibits a direct band gap of 3.66 eV [2] for thin films (determined from transmittance measurements) and of 4.42 eV [3] for nanoparticle assemblies. From the analysis of photoluminescence spectra, excited by radiation corresponding to fundamental absorption band of In₂O₃ layer, the energy band diagram of Sn and Cd impurity levels was determined. Energies of the levels induced by dopants and O atoms diffused in the interface InSe layer were determined from the analysis of photoluminescence spectra of InSe:Sn and InSe:Cd layers from In₂O₃/InSe interface. The (n- and p-InSe)/In₂O₃ structures display significant photosensitivity over a wide spectral range, from ultraviolet to near-infrared (Fig. 1). The influence of Cd and Sn concentrations on the

photosensitivity, mean free path and recombination rate of nonequilibrium charge carriers in n- and p-InSe layers from the InSe/In₂O₃ interface was also studied.

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T1-O Structural, optical and electrical properties of ZnO:Co,Ni thin films deposited by spin coating

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Nanocrystalline thin films of low Ni, Co doped ZnO were deposited onto quartz substrates by using a spin coating method. Post-annealings were performed at 450 °C and 650 °C. Structural and optical properties were investigated by using X-ray diffraction, X-ray photoelectron spectroscopy and UV-VIS. The surface morphology, roughness and piezoelectric properties were investigated by atomic force microscopy and showed the influence of dopant nature and annealing temperature. The codoping samples indicate a much higher thermal stability. XPS investigation indicates valence +2 both for Ni and Co. The optical properties were investigated in detail, the thin films being highly transparent. Our results revealed an influence of the Co and Ni doping level on the optical parameters of the ZnO thin film (the doping process leads to a decrease in the optical band gap). The investigations of the electrical properties revealed a decrease in the electrical conductivity in the doped samples.

Online

T14-PL: Nanoplasmonics and quantum metamaterials for room-temperature quantum photonics

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Plasmonic nanomaterials and quantum metamaterials have the unique ability to confine light in extremely sub-wavelength volumes and massively enhance electromagnetic fields. In the strong-coupling regime the energy exchange between the excited states of molecules/materials and plasmons is faster than the de-coherence processes of the system. As a result, the excitonic state of a quantum emitter can become entangled with the photonic mode, forming hybrid excitonic-photonic states. These plexitonic states are part light, part matter and allow for the characteristic Rabi oscillations of the atomic excitations to be observed.

Until recently, the conditions for achieving strong-coupling were most commonly met at cryogenic temperatures such that de-coherence processes are suppressed. As a major advance, room-temperature strong coupling has recently been observed using nanoplasmonic cavities and quantum metamaterials [1]. The fact that strong-coupling conditions may be reached at room temperature is of immense interest because it represents a clear route to a practical use of quantum effects in fields such

as bio-sensing and implementation of true quantum behaviour in quantum photonics [1].

The talk will discuss the principles of room-temperature strong coupling in nanoplasmonics and illuminate perspectives for quantum photonics. We will highlight recently demonstrated room-temperature strong coupling of single molecules in a plasmonic nano-cavity [2] and near-field strong coupling of single quantum dots [3] as well as strong coupling and exceptional points in active hyperbolic metamaterials [4] and graphene-based quantum metamaterials [5]. We will discuss the electron-beam control of plexitonic dynamics [6] and further present a new protocol demonstrating how nanoplasmonic room-temperature strong coupling offers an innovative route towards single-molecule immunoassay sensing [7] as well as enhanced single-photon emission and dynamic quantum entanglement [8].

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T2_PL: An original laser-based method for measuring the adsorption energy on carbonaceous surfaces

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The reactivity of carbonaceous surfaces bears a fundamental role in various fields, from atmospheric chemistry and catalysis to graphene and nanoparticles. This reactivity is mainly driven by the surface chemical composition and by the strength of the interaction between the adsorbates and the surface (physi-/chemi-sorption). Detailed, molecular-level chemical composition analysis of complex natural samples (e.g. combustion-generated aerosols) is usually performed by mass spectrometry methods in association with a surface-sensitive probe [1], while the adsorbate/surface binding is often overlooked. Continuing a series of works on the characterization of carbonaceous particles (soot) by two-step (desorption/ionization) laser mass spectrometry (L2MS) [2,3], we propose an original method for measuring the adsorption energy of aromatic molecules on their surfaces.

The method was validated on “surrogate soot”, i.e. a known (sub-monolayer) amount of polycyclic aromatic hydrocarbons (PAH) adsorbed on carbonaceous surfaces (HOPG, carbon black, etc.). Two variants of this method have been developed:

the “pulse-to-pulse decay” and the “fluence curve”. In the former, successive (nanosecond) laser pulses of constant energy are applied to the same desorption spot ($\sim 200\text{ }\mu\text{m}$ diameter), while in the later, various spots on the surface are probed with single pulses of increasing energy. In both cases, the desorbed neutral molecules are ionized by a UV laser and further detected by a time-of-flight mass spectrometer, hereby monitoring the signal of all adsorbates present on the surface. A pseudo-exponential decay is obtained in the “pulse-to-pulse” approach, whereas a monotonic increase towards saturation is returned by the “fluence” variant. These two different approaches complement each other and, when combined, help reduce the uncertainties induced by possible non-homogeneous surface concentration and/or fluctuations in laser fluence. The experimental data are fitted by a theoretical model completed by Bayesian statistics tools to extract the adsorption energy, either based on the assumption of quasi-thermal desorption of molecules (steady-state approximation) at low laser fluences [4], or, in a subsequent more refined model, considering the fast transient surface temperature profile upon laser irradiation. This was done by implementing a numerical approach based on a two-dimensional heat equation to calculate the space-time evolution of the surface temperature in the irradiated zone.

The proof of concept [5] of this original method has been performed with the adsorption energies of pyrene and coronene on black carbon, which are in good agreement with values reported in the literature. The extension of this method to “real” combustion-generated particles will be also presented.

The newly proposed method offers much wider application opportunities as it can be applied to a virtually unlimited number of adsorbates/surfaces combinations.

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T11-PL: Order Formation in Block-Copolymer Thin Films used for Lithography Nanomasks

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Block copolymer (BCP) lithography is an emerging technology aiming at the patterning of surfaces in the sub-10 to 20 nm range of minimum feature sizes, providing a low-cost/large-area alternative to conventional, light-based lithography techniques used in semiconductor device fabrication. BCP lithography is based on the self-assembly of microphase domains consisting of the individual polymer species making up either a binary or ternary BCP. Subsequent to the ordering process one of the polymer species of the BCP thin film is selectively removed, resulting in the formation of a nanomask

with mask openings the size and distance of which is dictated by the length of polymer strands forming the BCP. Thus, feature size in BCP lithography can be tuned by designing the length of macromolecules.

In order to allow for applications of such BCP films as nanomasks, however, not only the microphase separation but also the orientation of microdomains on a substrate surface needs to be controlled such that BCP domains are aligned laterally instead of vertically. This is typically achieved by neutralizing surface layers or by prepatterning the surface either chemically or morphologically, called chemo- or graphoepitaxy, respectively, or a combination of both. By this, accurate control on the position of mask features can be gained, even on a wafer scale.

In this presentation, recent progress in the understanding of order formation in block copolymer (BCP) thin films used for the fabrication of lithography nanomasks will be reported. The role of carefully tuning the total interfacial energy, i.e. the sum of all BCP internal and film external (to the substrate and the air) interfacial energies will be emphasized. State-of-the-art high-resolution TEM and STEM (Fig. 1) in combination with numerical image analysis tools will be employed among other techniques to reveal nanomask features on the sub-nanometer length scale. For the example of different polystyrene-polymethylmethacrylate (PS-*b*-PMMA) BCPs it shall be explored how complete the microphase separation will be and how mask opening sizes and the line edge roughness of resulting nanomasks depend on the selective polymer removal strategy

used. The insights gained are paving the way for applying BCP lithography for a big variety of nanopatterning tasks.

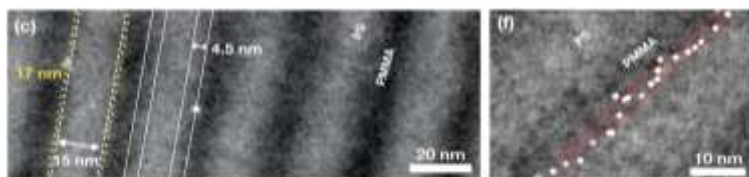


Fig. 1. STEM-ADF images of a lamellar PS-b-PMMA BCP film. [1]
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T1-PL: Silicon: Past, present and future

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Silicon is widely used in electronic industries in a number of forms, for example: amorphous silicon is used in liquid-crystal display units; polysilicon is used in Flash memory structures and photovoltaic solar cells; single crystals are used in C-MOS technologies etc. There are a few methods by which crystalline silicon is manufactured. Some of these manufacturing methods use a large amount of electricity and result in a large amount of carbon footprints. These methods also contribute to production of waste materials and greenhouse gases. My presentation will address the various silicon production methods for various applications and the need for alternative silicon production methods.

T6-PL: Plasmonic nanoplatforms - from fabrication to implementation in biomedical applications

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In this presentation we give an overview on our current approaches to fabricate, functionalize and integrate in biomedical applications a large variety of plasmonic and hybrid nanostructures exhibiting interesting spectroscopic, imaging and therapeutic capabilities. Nanostructured films fabricated using template-assisted assembling methods and chemically synthesized gold or silver nanoparticles of controlled size and shape (rods, prisms, stars-shaped) are designed to provide the right optical response for sensing and the required biocompatibility to be translated into specific in vitro and in vivo studies. For instance, a class of biocompatible “optically hot” nanoparticles stabilized by biopolymer coating (chitosan, poly(ethylene) glycol, pluronic, gelatine) were demonstrates as both spectroscopic intracellular imaging agents via surface-enhanced Raman scattering (SERS) and fluorescent lifetime imaging (FLIM) and versatile nanoprobe, drug delivery carriers and plasmonic-induced hyperthermia agents. Scanning confocal Raman microscopy combined with dark-field and confocal fluorescence microscopy were used to record relevant information about nanoparticle localization, intracellular chemical interaction and pH mapping. In recent years, our

research group has provided several “proofs of concept” of therapeutic mechanisms based on combined plasmon-induced photothermal therapy (PTT), photodynamic therapy (PDT) and nanochemotherapy [1,2]. Currently, we focus on the development of new nanoplatforms for multiple NIR light-activated nanotherapies as well optical imaging contrast agents for NIR real-time image-guided surgery of cancer.

Acknowledgements. This work was supported by a grant of Ministry of Research and Innovation, CNCS-UEFISCDI, project number PN-III-P4-ID-PCCF-2016-0142, within PNCDI III.

Poster Session & Coffee Break

HALL 1

T5-P: Chemiresistors based on nanostructured heterojunctions of Copper and Titanium oxides doped by Lithium

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Gas sensors based on thin films of CuO-TiO₂ heterojunctions doped by Lithium were synthesized by a 2-step method: (i) repeated ion beam sputtering of the building elements (on the Si substrates and multisensor platforms), and (ii) thermal annealing in flowing air. Active films were deposited on

chemiresistor substrates KBI2 (Tesla Blatná). Properties of films were studied by SEM and AFM. Prepared films are exhibiting a p-type conductivity. Sensitivity of prepared chemiresistors to gaseous analytes was evaluated using a specific lab-made device operating in a continuous gas flow mode. The obtained results showed that the Li doping significantly increased the sensitivity of the sensors to oxidizing gases, such as NO₂, O₃, and Cl₂, but not to reducing H₂. The sensing response of the CuO-TiO₂-Li chemiresistors improved with increasing Li content. Doping CuO-TiO₂ sensing films with Lithium improve sensing response 4 times in case of NO₂, and almost two orders of magnitude in case of O₃ and Cl₂. For the sensors with about 15% of Li at., the detection limits were as follows: NO₂ → 0.5 ppm, O₃ → 10 ppb, and Cl₂ → 0.1 ppm. The Li-doped sensors showed excellent sensing performance at lower operating temperature (200 °C), however, even though their response time was only a few minutes, their recovery was slow (up to a few hours) and incomplete. The results showed that the CuO-TiO₂-Li based chemiresistors are promising for the detection of oxidizing gasses.

T6-P: Magnetic properties and magnetocaloric effect in La_{0.7-x}Eu_xBa_{0.3}MnO₃ and La_{0.7-x}H_xBa_{0.3}MnO₃ nanoparticles.

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Structural, magnetic properties and magnetocaloric effect of La_{0.7-x}Eu_xBa_{0.3}MnO₃ and La_{0.7-x}H_xBa_{0.3}MnO₃ nanocomposite powders have been investigated. The compounds were produced by Sol-Gel method. The structural and morphological properties were investigated by X-ray diffraction and

Transmission Electron Microscopy, respectively. Both measurements show that the average size of the nanoparticles is 40-50nm and lattice parameters obtained from XRD measurements tend to slowly diminish with increased doping level. Magnetic measurements were done using Vibrating Sample Magnetometer in the range 4-300K and display ferromagnetic order below T_c and systematic decrease in T_c caused by doping. Magnetic enthalpy change was determined from magnetic isotherm measurements for each compound. Plots present a wider range in temperature in effective magnetocaloric effect with a lower peak compared with bulk material. Relative cooling power was calculated. Comparison and advantages of nano-particles over bulk is discussed further.

T8-P: Fluorene-based chemical tools for light-emitting materials

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Organic light-emitting diodes are envisaged to evolve as the next-generation lighting sources due to superior behavior in terms of mechanical, thermal, and chemical stress as compared to inorganic counterparts. Materials-enabled innovation enables higher color quality/tunability and unlocks ultrathin, large area, flexible displays. Conjugated polymers are the key players in the field and polyfluorenes the archetypical "blue" emitting polymer [1]. This prominence is driven by their unique molecular structures and commercially relevant properties (efficient emission, excellent electronic traits, facile synthesis

and molecular tailoring, suitable processing) [2]. However, the reliable polyfluorene system still needs improvement (major issue: photo- or electro-oxidative degradation) and the development of new building blocks is a key challenge [3]. Optimization of synthetic pathways is another issue since preparation protocols are often conducted only to achieve optical features already available at short chains. Nevertheless, materials' behavior can be extremely sensitive to the length of the polymer chains, and a polymer-based device will finally fail if it softens, fuses or cracks under operating conditions. This work exploits the potential of Suzuki polycondensation to gain mechanistic insights and generate polyfluorenes with high molar masses and relevant optical behavior (blue emission, high quantum yield), based on new fluorene building blocks decorated with short alkyl chains displaying polar nitrile or amino terminal functionalities. These particular monomers generate a suitable protection against collisional quenching of fluorescence and enable future post-polymerization modifications, like quantitative deprotection and the attachment of subsequent electroluminescent moieties.

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T8-P: Silicone-spin crossover composites capable of multi-stimuli response

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This work reveals the possibility of extending the applicability of silicone elastomers by combining the excellent properties of silicone elastomers with those of spin-crossover complexes (SCO). Spin-crossover materials (SCO) are capable of undergoing reversible switching between two electronic configurations (low spin - LS and high spin - HS) upon application of external stimuli, such as temperature, pressure, light, pH, electric and magnetic field.[1,2] SCO material plays a dual function when incorporated into the silicone elastomer: enhance the dielectric permittivity and induce sensitivity to new stimuli. For morphological characterization, the composite films with various concentrations of SCO material were submitted for SEM analysis in cross section. The presence of SCO material in the PDMS matrix led to an increase of dielectric permittivity from about 3 for neat PDMS to almost 8.5 for composite with 50 wt% SCO. The tensile tests showed that the strain at break for all composites is higher than 300 % and decrease with increasing the concentration of SCO. The ability of these composite materials to respond to different stimuli was assessed by specific analyzing techniques such as electromechanical actuation and temperature dependence of magnetic, electric and optical properties.

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T8-P: Composite materials obtained by the recycling of construction and demolition wastes

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Construction and demolition wastes represent a half of the total amounts of solid municipal wastes generated in the world, occupy large storage spaces and cause pollution which becomes a serious problem nowadays. The scientific research in the field was focused on the recycling of construction and demolition wastes for the production of concrete, cements and bricks. The obtaining of these products was limited to the addition of suitable binder contents such as lime or cement, compaction and possibly heat treatment, without to be a concrete recycling method. On the other hand, till date, ferrites have captured the attention of scientific communities because of their excellent magnetic, biocompatible and catalytic properties. These properties are largely dependent on their dimensions and as result synthesis of uniform nanoparticles is extremely important because compared with bulk size, the conductivity and electronic structure change dramatically. By the continuous improvement of traditional synthesis methods, new synthesis techniques must keep emerging to meet better performance [1]. The aim of this paper is: i) to recycled the construction and demolition wastes, namely broken glasses,

iron and cast iron wastes, by a new, simple, low cost and environmental friendly method and ii) to investigate the structure of the new recycled materials in view of applications. Up new, this synthesis method do not described in the literature for the obtaining of ferrites. The recycled materials were characyterized by: XRD, SEM, FTIR, UV-Vis and EPR spectroscopy. The XRD data indicate vitroceramic structures with varied crystalline phases. A simple inspection of the SEM micrographs reveals that the composite material containing a large amount of iron wastes has a slightly better homogeneity while for the material doped with cast iron waste the morphology ie heterogeneous, with cracks and random cristalinity. The ferrite phases, namely Fe_3O_4 and MgFe_2O_4 crystalline phases, were detected in the composites containing the iron wastes. By doping with different contents of iron wastes were evidenced structural modifications in the silicate network and in the process of water absorption.

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T8-P: Comparative structural, morphological and optical characterization of CeO_2 /doped- CeO_2 nanoparticles

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In the continuous progress of society, the problem of water pollution has becoming increasingly severe, especially due to the degradation-resistant organic pollutants potentially hazardous to environment and human health. In comparison with traditional methods (adsorption, sedimentation or filtration), characterized by high energy consumption and low efficiency, photocatalysis provides multiple advantages, namely

the ability of complete mineralization of the pollutants under ambient temperature and pressure, efficiency, nontoxicity or cost-effectiveness in the degradation of organic pollutants. Among the proposed materials, metal oxide nanoparticles (TiO_2 , ZnO , CeO_2) demonstrated their vast photocatalytic potential, especially under UV irradiation. However, the intrinsic wide bandgap of these NPs represents a major drawback generated by the inefficient utilization of solar energy, which limits their further use in real environmental pollutant treatment. In order to shift the photocatalytic performances of metal oxide NPs towards visible and infrared region of solar light, various approaches have been reported, such as doping, coupling with other semiconductor material or surface modification. CeO_2 nanoparticles were reported as efficient photocatalysts with improved attributes as compared with TiO_2 NPs, due to their high oxygen storage ability, eco-friendly properties and photostability. In this context, the present paper will describe the synthesis of CeO_2 NPs by means of various preparative methods, followed by their methodical characterization in order to evaluate their structural, morphological and optical attributes. Also, aiming the translation of photocatalytic activity to visible light, the preparation of some Co-doped CeO_2 samples will be reported, highlighting the differences between the samples.

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T8-P6 Hierarchical biointerfaces obtained by laser processing and surface functionalization for tissue engineering

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The potential of Mesenchymal stem cells (MSC) for implantology and cell-based therapy represents one of the ongoing research subjects within the last decades. In bone regeneration applications, the various environmental factors including bioactive compounds such growth factors, chemicals and physical characteristics of biointerfaces are the key factors in controlling and regulating osteogenic differentiation from MSCs. In our study we have investigated the nano and micro hierarchical biointerfaces influence on the osteogenic fate of MSCs. The complex interfaces were created via a laser texturing technique and peptide surface functionalization. Scanning Electron Microscopy, EDAX, contact angle and surface energy of the analyzed coatings were correlated to biological response on both short and longer term (72h, respectively 28 days). Human MSC were cultured on the developed coatings and viability, proliferation and morphology were evaluated. All surfaces were shown not to exhibit toxicity, as confirmed by LIVE/DEAD assay. Micro and nanotextured ceramic interfaces exhibited an increase in osteogenic differentiation of hMSC cells, results supported by ALP and mineralization assays. This is the first report about nano and micro hierarchical biointerfaces based

on ceramics directing osteogenic differentiation from hMSCs indicating the potential for application in bone regeneration.

T10-P: Monitoring spin-crossover properties by diffused reflectivity

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Spin crossover (SCO) materials exhibit a spin transition between a low-spin (LS) and a high-spin (HS) state which can be induced by an external stimulus such as temperature, pressure, magnetic and electric field or by light [1-2]. During the spin transition, the SCO complexes undergo drastic changes of their physical properties, allowing for the design of smart devices with tunable magnetic, electrical, dielectric or optical response. Due to the color change that usually accompanies the spin transition, the fraction of complexes in the high-spin state has frequently been monitored by optical measurements using diffuse reflectivity as many of these compounds are obtained in the form of powders [3-4]. In the field of spin transition solids, the first reflectance studies assumed a linear dependence of

the remittance with the fraction of complexes in a given spin state. However, very often the reflectance measurements did not fully reproduce the data obtained from alternative techniques, for example magnetic susceptibility data. In early literature, these differences were omitted or attributed to the fact that the reflectance data are collected from the surface of the sample while the magnetic measurements gives access to the volumetric behavior of the sample. If in some cases, for example in the analysis of the major hysteresis loop, these differences between optical and magnetic data does not change the interpretation of the physical phenomenon, it is no longer the case of the more intimate properties, such as relaxation behavior or inter-domain interactions of the spin-like domains, where the raw reflectance data can lead to wrong conclusions. In this work we present a detailed study showing the importance of the Kubelka-Munk (KM) correction [5] in the analysis of diffuse reflectivity measurements to characterize spin crossover compounds. Combined reflectance and magnetic susceptibility measurements are carried out as a function of temperature or time to highlight the conditions under which this correction becomes critical. In particular, we investigate the influence of the color contrast between the two spin states on the reflectance measurements [6].

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T10-P: The characterization of enzyme-polymer hybrid interfaces obtained by MAPLE for sensor applications

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Obtaining hybrid enzymatic-based interfaces for sensing application require the use of a multiuse, reusable sensor. By controlling the interface characteristics in terms of the surface chemistry, thickness, and roughness, a tailored response toward various toxic compounds can be obtained, regarding both materials used as active surfaces and fabrication methods. Herein, we report a preliminary study on using a laser-based method (i.e., matrix-assisted pulsed laser evaporation, or MAPLE) for obtaining active polymeric-enzymatic interfaces as hybrid coatings for sensors applications. The MAPLE fabrication consisted of the simultaneous alternating evaporation of layers of polyethylenimine (PEI) and enzymes. The deposition processes of the polymer and enzyme were carried out using a double-target system and a Nd:YAG pulsed laser, operating at 0.45 J/cm² fluences with a wavelength of 266 nm and a repetition rate of 10 Hz. Fourier transform infrared spectroscopy revealed no significant changes in the functional groups of both hybrid and layered coatings compared with the initial material. The thickness and roughness, as well as the morphologies of the coatings were analyzed by atomic force microscopy and scanning electron microscopy.

T10-P: Studies on graphene/PEDOT:PSS and graphene/polysiloxane composite layers

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Graphene-based polymer nanocomposites have many applications in various domains and are strongly dependent on the dispersion of the two components within the composite structure. In this study we show some experimental results obtained on graphene flakes/polydimethylsiloxane and graphene/PEDOT:PSS nanocomposite layers.

The structural, morphological optical, electrical and magnetic properties of the nanocomposites with different graphene and silica contents were studied using XRD, SEM, Raman, FTIR, XPS, UV-VIS and EPR methods.

It was established that the physical properties of nanocomposites are controlled by interfacial interactions, agglomeration and exfoliation of the filler. The addition of SiO₂ nanopowder could play a role in the exfoliation process of graphene flakes into the polymer matrix.

T14-P: Integration of RFID with diffractive optical elements in multi-layer security labels

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We propose a multilayer structure fabricated with a low-cost technology that offer the possibility of obtaining holographic labels with two different sets of security elements integrated with RFIDs for increased product protection against counterfeiting. The first layer is a diffractive background designed with specific software, meanwhile the second one is a nanotext impossible to identify with the naked eye. To attain the desired structure the two security elements are obtained by double UV exposure and a single development process. The nanotext is placed at specific untraceable coordinates on top of the diffractive optical elements (DOE) and represents the foreground of the label. To increase even more the level of security offered by these types of labels, an RFID element is incorporated in order to monitor the product in the logistical warehouse and insure the protection against counterfeiting. The device structure is given in Fig. 1.

In Fig. 2 one can see an image with the holographic background, an optical image of the nanotext security element, and an AFM scan detailing the placement of the additional security elements on top of the background composed by DOE arrays.

This multilayer holographic label can be used to check the authenticity of a large variety of products during the distribution process.



Fig. 1. Structure of the multi-layer security label

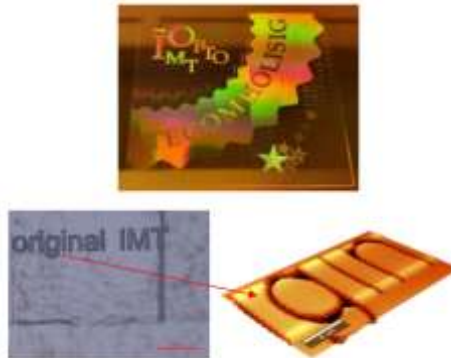


Fig. 2. Security label DOE background with nanotext details

A high level of protection is achieved by employing two individual designers, one for DOE background with different visual effects and another one for nanotext's shape and coordinates. An additional security level is introduced by the RFID.

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Poster Session

Online

T6-P: Intrinsic photoluminescent protein-stabilized gold nanoclusters: towards fluorescence imaging applications

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Herein, we developed bovine serum albumin stabilized gold nanoclusters (BSA-AuNCs) with an intrinsic photoluminescence emission in the first biological window, performing as efficient contrast agents for in vitro and ex vivo imaging applications. According to transmission electron microscopy, the as-synthesized BSA-AuNCs agents, exhibiting intense and stable photoluminescence around 670 nm, consist in protein polymerized-chains dopped with AuNCs with an average size of 2–3 nm. Next, the photostable BSA-AuNCs were functionalized with folic acid (FA-BSA-AuNCs) in order to achieve an active targeting of NIH:OVCAR-3 human ovarian adenocarcinoma

cells, towards bioimaging applications. The improved cellular uptake and staining ability of FA-BSA-AuNCs compared to the BSA-AuNCs was validated by fluorescence imaging microscopy under one-photon excitation. Finally, we demonstrate the ability of BSA-AuNCs to perform as reliable bright and photostable contrast agents for the visualization of cancer tissue mimicking agarose-phantoms using fluorescence lifetime imaging microscopy approach under non-invasive two-photon excitation. Considering their valuable fluorescent properties, BSA-AuNCs show great promise as efficient contrast agents towards image-assisted tumor surgery. This work was supported by CNCS-UEFISCDI, Project PN-III-P4-PCCF-2016-0142.

T6-P: Spectroscopic insight into the optical properties of ZnO nanoparticles synthesized by simple chemical methods

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ZnO nanoparticles (NPs) show numerous possible applications in the fields of sensors [1], opto-electronics, or photocatalysis [2]. Here, we investigated the size dependent structural, optical, and vibrational properties for ZnO NPs of various sizes and shapes, synthesized using simple, cost-effective chemical methods. All samples exhibited a strong UV absorption band in the 330-370 nm spectral region depending on the particle

diameter and intense UV emission, followed by two visible emissions (blue and green) of smaller intensities. The intensity ratio between the UV and visible emission bands showed an increase with the particle size. A decrease of the green emission was observed for the ZnO samples that presented both EPR signals, compared to those that showed only the $g=2.005$ EPR signal.

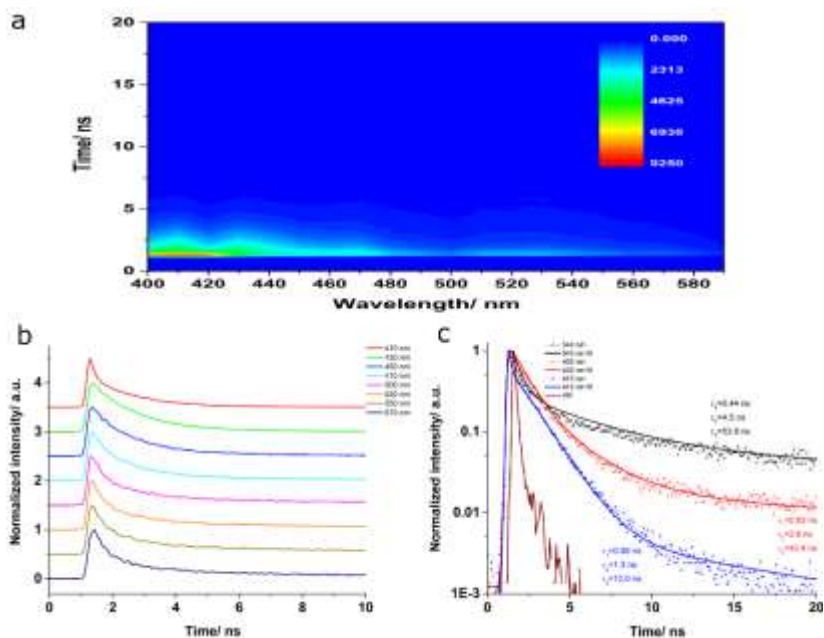


Fig.1. (a) Time-correlated single photon counting (TCSPC) data obtained from ZnO flower-shaped NPs of 7.9 nm diameter, upon excitation at 340 nm; (b) Selected decay profiles at various emission wavelengths (c) The decay profiles with fitting curves

The time-resolved fluorescence investigations revealed three different dynamics: a fast one in the 400-430 nm spectral

region, assigned here as the UV band-tail region, a middle one in the blue region of the spectrum (440-470/480 nm), and a longer one in the green spectral region (Fig. 1) [3].

The lifetimes obtained for the decays in the visible and blue emission spectral ranges, respectively, presented an overall decrease with increasing the particle diameter, in accordance with the observed energy band-gap inverse dependence on particle diameter. The faster decay components obtained with increasing the particles size may indicate the presence of more active sites for the transfer of electrons, such as inherent defects of electron vacancies, which could appear due to particle growth. Ongoing research is focused on developing these ZnO NPs for surface enhanced fluorescence and surface enhanced Raman scattering applications. Preliminary results will be presented.

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T8-P: Assessment of Us-Up Equation of State Parameters for Silicone Elastomers

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Starting with the late 90's the dielectric properties of silicone based elastomers have been rediscovered paving the way for applications such as flexible electrical capacitors [1]. This circuit elements work like rigid capacitors from an electrical point of view but under Maxwell stress may function as actuators. When mechanical load is applied, the capacitors change their capacitance, and may be used as sensors. Taking advantage of the latter effect, sensors may be developed to function as strain gauges in places where the accessibility is restrained and high-resolution readings are required. In civil engineering, and especially geotechnical engineering, monitoring strains with low-cost sensors, may be the key to evaluate the distribution of stresses along soil-structure interfaces. The current monitoring systems for tunnels, or retaining structures consists of expensive and bulky equipment. Using silicone dielectric elastomers we propose the development of low-cost sensor arrays for assessing the distribution of stresses between structural elements. The study shows the steps being taken for obtaining the mechanical parameters necessary for numerical modelling of the planar flexible capacitors, taking into account that such an approach is necessary for the evaluation of the sensor geometry for each type of application. The complexity of the numerical models reside in the quasi-liquid mechanical behavior of the solid state cross-linked silicone elastomers. The behavior of the material is described by Mie-Gruneisen equation of state (Us-Up) in it's linear form (Hugoniot). The parameters for this equation have been assessed using a Charpy-like impacting device, developed for applying low-velocity shockwaves to the material in order to match the range of the actual loading of the sensor.

[1] D. Grady, Physics of Shock and Impact Volume 1, Fundamentals and Dynamic Failure, IOP Publishing Ltd., 2017.

T8-P: Improved piezoelectric property of PVDF by ZnO nanostructures incorporation

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Polyvinylidene fluoride (PVDF) is an environmentally friendly piezoelectric polymer and its piezoelectric properties need to be enhanced. In this study, we obtained high percentage of polar β and γ crystallographic phases (responsible of its electroactive properties) in PVDF through solution casting method without any mechanical or electrical treatment. Pristine PVDF and ZnO/PVDF nanocomposites were prepared by casting solutions of PVDF (in acetone/ dimethylformamide) and applying heat treatment between 50 and 100 °C. Also, ZnO nanoparticles or small nanorods were added in PVDF solutions before casting to form composites films. The structural and morphological changes were investigated through X-ray diffraction, Raman spectroscopy, Fourier transform infrared spectroscopy, scanning electron microscopy, and atomic force microscopy. The effect of PVDF concentration, solvents ratio and temperature of thermal treatment on the crystallization of α , β , and γ phases of PVDF from casting solution was studied. Also, the modifications in structure and properties of composites induced by the presence of ZnO nanostructures were investigated. The content of piezoelectric β and γ phases was increased with ZnO addition, probably due to the fast nucleating or catalytic effect of the wurtzite crystals. The results

indicate that PVDF/ZnO composite coatings can be used for the fabrication of piezoelectric devices.

T8-P: Effect of the hybrid filler on properties of recycled polypropylene-based wood-plastic composite

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Recycled polyolefins are among the major components of global municipal solid waste, which are often burned and landfilled, while they present a promising raw material source for producing wood-plastic composites (WPCs) due to their large volume and low cost [1, 2].



Fig.1. The sewage sludge isolated after centrifugation and the air-dried sludge

A sewage sludge (SL) isolated from wastewater of the hydrothermal treatment of wood for plywood production by coagulation/flocculation modes is also of interest for usage as a secondary raw biomass material. In this work, the sewage sludge was isolated from the wastewater with the developed complex coagulant (Fig. 1) and used together with birch sawdust microparticles (BSM), activated with a dilute sodium

hydroxide solution at 90°C during 5 h, as a hybrid filler in the WPC based on recycled PP.

Its content in the composite samples did not exceed 30%. The samples were obtained by mixing recycled PP, the birch sawdust and the air-dried separated sewage sludge in a high-speed mechanical mixer, than the mixture was dried at 60°C during 48 h, and then it was processed by the extrusion and molding methods.

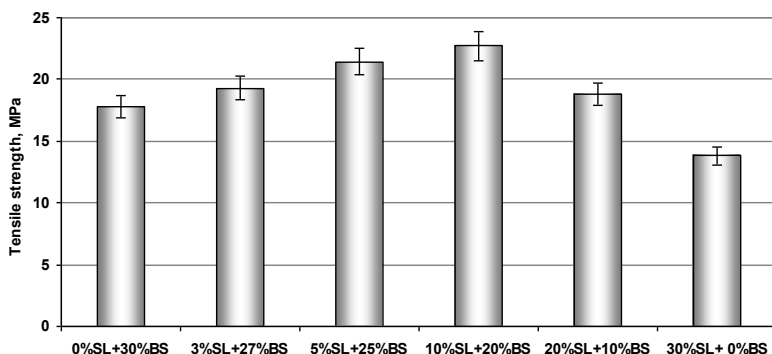


Fig. 2. Effect of the sewage sludge on tensile strength of the WPC samples

The obtained WPC samples with the hybrid filler showed the increase in mechanical strength (Fig. 2) and contact angle values, and the decrease in water sorption and swelling degree at the content of the sludge less than 10%. However, the subsequent increase of the sludge content more than 10% led to the deterioration of the properties of the WPC samples.

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- [2] G. Shulga, B. Neiberte, J. Jaunslavietis, A. Verovkins, S. Vitolina, S. Livcha, *Bioresources* 16(2) (2021), 2804-2823.

T8-P: Comparison of electron-beam irradiated polymers

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When evaluating the behavior of a polymer material in a given working environment, one must take into account the particular dynamic nature of polymers, compared to other materials, due to their complex 3D structure, where both the chemical unit and the macromolecular chain play important roles. Thus, polymers present intrinsic internal mobility and any bulk or surface perturbation of the material may affect its mechanical and physico-chemical properties.

Several methods can be used to induce modifications of a polymer material, in order to assess and control the evolution of the bulk and surface properties. Thus, the molecular structure of polymers and consequently their properties can be significantly modified by electron beam irradiation. The main reactions during the irradiation process are chain scission, chain branching and cross-linking. Taking this into account, here the influence of electron-beam irradiation on low-density polyethylene (LDPE), polystyrene (PS) and poly(methyl methacrylate) (PMMA) was investigated. The three polymers, belonging to the carbonchain polymer class, allow a comparison between non polar, as PE and PS, and polar structure, as PMMA, and bear other differences in their structure, since PS presents pending aromatic groups and is amorphous, same as PMMA, whereas LDPE has only hydrogen

atoms bonded to each carbon atom and is semicrystalline. Also, PMMA has an important oxygen content in its structure.

The irradiation was carried out under mild conditions, in order to identify the effects that may dominate in a given polymer, depending on several factors, such as the chemical structure and morphology of the polymer, as well as the irradiation conditions and the post-treatment.

The chemical properties of the polymers were monitored combining Fourier-transform infrared (FTIR) and X-ray photoelectron spectroscopy (XPS); the modifications in the crystalline/ amorphous structure were assessed by X-ray diffraction (XRD); the viscoelastic behavior was analyzed using dynamic mechanical analysis (DMA). Supplementary, the surface was tested by contact angle measurement.

The XPS analysis shows that the untreated LDPE and PS samples present intrinsic low-level oxidized carbon atoms, which may reasonably be attributed to carbon singly bonded to oxygen. This result is not surprising for commercial polymers. Interestingly, after irradiation all these functional groups are removed from the structure and no oxygen is detected by XPS. Also, the oxygen content of PMMA presents a certain decrease. The removal of oxygen may imply chemical reactions conducting to the creation of radicals, which, on one side, may link to each other in the bulk and develop a crosslinked structure. On the other side, these radicals may behave differently at the surface, inducing a polar surface character. This is sustained by the water contact angle values, revealing an evolution from hydrophobic to slightly hydrophilic on LDPE and PS, and also an increase of the hydrophile character for PMMA.

Then, the mechanical properties of the polymers, investigated in (–150 to 200°C) temperature range, show that the effects of the irradiation are small, but detectable. Thus, there is some increase in the storage modulus and the glass transition temperature, which would imply some reduction in the mobility of the macromolecular chains, due to crosslinking.

The electron-beam irradiation of polymers, conducted under mild irradiation conditions, has as dominant effects the creation of radicals and crosslinking. The effects are similar for the tested polymers, although these have different chemical structure and morphology. The crosslinked structure reinforces the rigidity and hardness of the material.

T8-P: Raman microscopy and spectroscopy studies of graphene nanoplatelets/low density polyethylene nanocomposites materials

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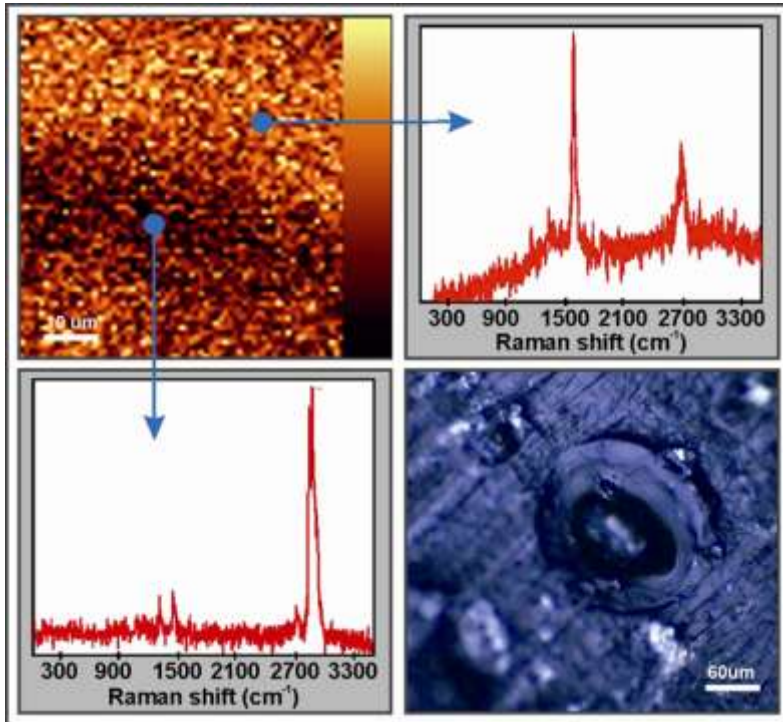
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Composites consisting of low-density polyethylene (LDPE) and graphene nanoplatelets (GnPs) of various concentrations were developed by mixing methods, using the nanoplatelets in molted polymer and dispersed forms of the polymeric matrix respectively and their structural and morphological properties were studied. As known, the properties of the composites are determined by the graphene platelets content and control of

their properties can be achieved by the addition of graphene. The effect of composing on the properties of LDPE was thoroughly examined by Raman spectroscopy. Raman imaging was used as a non-destructive method for the spatial quantification of the mixing process of graphene and the polymer matrix.



In particular, the materials compositional homogeneity was studied using Raman spectroscopy, while, compositional mapping of the surface was done by Raman microscopy. These results were compared with scanning electron microscopy images. As shown, the GnPs concentration seriously affects the composite forming and can be correlated with electrical and mechanical properties of the new materials. Example of a

Raman microscopy map of the G (1580 cm⁻¹) and G' (2800 cm⁻¹) line positions of the 1.5% graphene containing composite material and corresponding spectra in two different points on the surface. The last is the optical microscopy image of the charted region of the sample.

T11-P: Analytical high-resolution STEM investigations of interfacial widths and line-edge roughnesses in microphase separated cylindrical block copolymer thin films

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Block copolymer (BCP) self-assembly (SA) is an emerging tool for the creation of ordered nanoscale features on large surface areas with controllable motifs and feature sizes in the 10 nm regime rendering a competitive alternative to conventional lithography techniques applied in semiconductor industries and beyond. BCP SA is based on the microphase separation of two blocks of immiscible polymer species, which are covalently bond to each other in a BCP chain. After selectively removing one of the blocks, a mask with e.g. hexagonally arranged pores is obtained. This mask can be used for further lithographical processes. Features after processing are a direct replica of their

lithography mask and can only be as precise as their templates. Thus, the quality of patterns obtained, e.g. the precision of nanostructures and their line edge roughness (LER) plays an important role, which is also strongly depending on the self-assembly process and abruptness of microphases in the BCP film. Additionally, the influence of subsequent removal of one polymer phase is equally crucial, yet insufficiently investigated. Utilizing advanced analytical (scanning) transmission electron microscopy ((S)TEM) techniques at 60 kV acceleration voltage, we provide real space information on polymer domain size and morphology, as well as the interfacial width and LER between polystyrene (PS) and polymethylmethacrylate (PMMA) in cylinder forming BCPs along the lithography process. To this end, membranes of untreated as well as wet chemically UV/acetic acid treated and Ar/O₂ plasma etched BCP thin films microphase separated on a sacrificial SiO₂ layer with an additional random copolymer brush for surface neutralization are prepared for the TEM by HF etching and skimming of the BCP film with a gold TEM grid. Domain sizes, interfacial widths and LERs (Fig. 1) are obtained by a self-written MATLAB application allowing for the analysis of angularly resolved radial intensity profiles of each individual pore in annular dark-field (ADF) STEM images. The mean radial intensity profile of the pore shown in Fig. 1(a) is displayed in Fig. 1(b).

The as-phase separated film exhibits a domain size of (11.8 ± 3.1) nm, an interfacial width of (5.2 ± 1.1) nm and a LER of (3.2 ± 1.5) nm between the PS matrix and the PMMA cylinder. After the UV light/acetic acid treatment the pores are significantly larger with a diameter of (19.1 ± 1.4) nm exhibiting

a much much-decreased diameter distribution. In addition, a reduced LER of (0.8 ± 0.6) nm and a strongly reduced interfacial width of (2.8 ± 0.7) nm is observed. The pores inside the O_2/Ar plasma dry etched films have a diameter of (24.7 ± 1.6) nm, and further reduced interfacial width of (1.6 ± 0.2) nm and a LER of (0.5 ± 0.2) nm, rendering this a possible candidate for high resolution lithography processes.

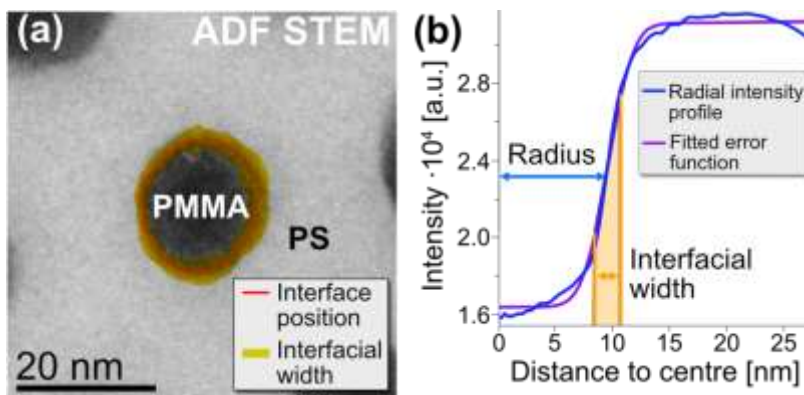


Fig. 1. (a) Evaluated ADF STEM image of a BCP with Interface position (red) and interfacial width (gold). These parameters are obtained from angularly resolved intensity profiles exemplarily shown in (b).

Further investigations by energy filtered TEM show that the thickness of the PS mask is reduced, and at sufficiently long treatment time PMMA is completely removed leaving nanoholes inside the PS matrix. Furthermore, an enhanced oxygen content is observed for the plasma treated film. Findings are confirmed by X-ray photoelectron spectroscopy (XPS) and polarization modulated infrared reflection absorption spectroscopy (PM-IRRAS).

T11-P: Order and arrangement of block copolymer domains in metallic antidot films

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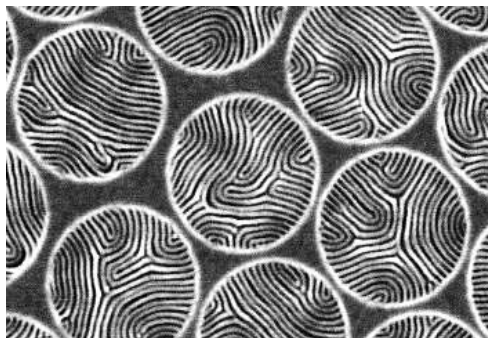
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Block copolymer (BCP) lithography is a well-established technique for economical large-area surface nanopatterning exploiting the microphase separation of a copolymer, here poly(styrene-*b*-methymethacrylat) (PS-*b*-PMMA) BCP into self-assembled nanostructures. Using a block length ratio of these two chemically different polymers of 50:50 we achieve perpendicular aligned lamellars with an width of 11 nm.

In order to guide the lateral alignment of these lamellar domains, we prepattern the substrate using nanosphere lithography (NSL). To this end the convective self-assembly of polystyrene nanospheres in a colloidal suspension is used to create an array of hexagonally closed packed spheres. These spheres are shrunk by reactive ion etching (RIE) and used subsequently as a shadow mask in a metal thin film deposition. After removal of the spheres an array of hexagonally arranged holes with an certain diameter is left in the metal thin film (antidot film). This is used as a prepattern for the BCP lithography.



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Fig. 1 Scanning electron microscopy image of an antidot patterned metal film on silicon, selectively filled up with a PS-*b*-PMMA BCP film forming a fingerprint pattern of lamellas perpendicular to the substrate. The PMMA phase is removed and the sample is coated with a thin Cr film to enhance image contrasts.

We demonstrate that using such prepatterned films the alignment of lamellar BCP domains can be controlled and tuned by adjusting the geometry of the antidot film like the film thickness and the diameter of the circular shaped holes. Furthermore, we can control locally the orientation of the polymer domains by adjusting the deposited amount of polymer in these metallic holes which allows us to change the orientation of the polymer domains from perpendicular to parallel to the surface. Finally we show that the alignment of these polymer domains follows also the morphology of the prepatterned substrate according to the film thickness, which can also be controlled, to achieve an desired alignment of nanometric features.

T11-P: XPS study of the selective removal of PMMA from nanophase separated PS-*b*-PMMA thin films

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Block copolymer (BCP) nanolithography is an emerging, competitive alternative to conventional lithography because it enables sub-10 nm features at low processing costs. In order to optimize nanostructure precision and morphology both the order formation in BCP thin films and the selective removal of one of the polymer blocks need to be well controlled. Among many BCP materials which are available today for BCP lithography polystyrene-*b*-polymethylmethacrylate (PS-*b*-PMMA) is the most commonly used polymer. Depending on block length ratios, either cylindrical (Fig. 1), spherical or lamellar nanopatterns can be created. PMMA can be removed selectively by different methods, leaving behind a nanopatterned PS mask. The aim of this study is to investigate the effectivity of different PMMA removal strategies, including reactive ion etching (RIE) or a combination of UV-irradiation followed by etching in acetic acid. The question is if a complete

PMMA removal can be achieved and if parts of the PS are removed at the same time. Moreover, the size and shape of resulting PS nanomask openings needs to be controlled. X-ray photoelectron spectroscopy (XPS), polarization modulated infrared reflection absorption spectroscopy (PM-IRRAS), scanning electron microscopy (SEM), scanning transition electron microscopy (STEM) and ellipsometry are used to study changes in morphology and surface chemistry during mask processing. The same techniques are also applied to study changes in random copolymer PS-*r*-PMMA films which are typically used as a neutralizing thin film at the BCP - substrate interface.

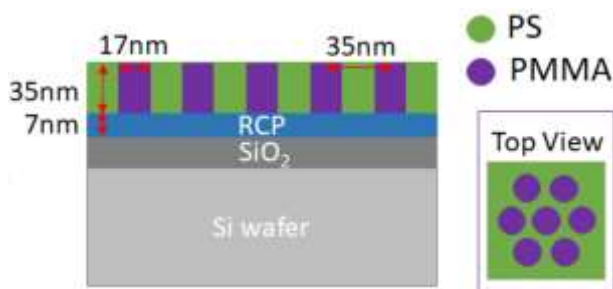


Fig. 1 Schematics of a nanophase separated PS-*b*-PMMA block copolymer. The RCP film also consists of styrene- and methylmethacrylate units. For high-precision nanopatterning it is required to remove PMMA and RCP selectively.

T14-P: Very Large Enhancement of the Optical Limiting Efficiency and Broadband Operation of Defect Engineered Graphene Oxides

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Recently, lasers have been extensively employed in both civilian and military fields for various applications.[1] However, an intense laser beam can potentially bring about human retinal injury and damage to delicate optical devices. As a result, many efforts have been devoted to developing highly efficient optical limiting (OL) materials that focus on preventing permanent damages from accidentally laser irradiation.

Graphene oxide (GO) is an efficient platform for designing tailor-made OL materials by defect engineering. In that view, the present work reports on the effect of defect-engineering of some reduced GOs on their OL action. Especially, the OL action of B, N individually doped (B,N-GO) and, B and N domain doped (BN-GO) GOs was systematically studied in the spectral region 450-2300 nm, using 4 ns laser irradiation.

The variation of the optical limiting onset values, OL_{on}, of B,N-GO and BN-GO dispersions for different irradiation laser wavelength is shown in Figure 1. As shown, the OL action for wavelengths up to 1100 nm remains practically unchanged. In this region, the OL_{on} values of B,N-GO and BN-GO were found to be rather constant and ~0.06 and ~0.07 J cm⁻², respectively.

However, towards longer NIR wavelengths, a continuous improvement of the OL efficiency was observed up to about 1700 nm, reaching OLon values as low as 0.001 and 0.002 J cm⁻² for B,N-GO and BN-GO, respectively. Moving to longer NIR wavelengths, the OL action was found to attain a plateau, remaining practically constant. Such low values of OLon correspond to record low values, to the best of our knowledge. It should be mentioned that the OL action of B,N-GO was found to be slightly better than that of BN-GO for all the irradiation wavelengths, most probably because it has more sp²-sp³ interfaces compared to BN-GO.[2] In general, defect-engineered graphenes with more sp²-sp³ interfaces are expected to exhibit strong OL action, as discussed elsewhere.[3]

The findings indicate the efficiency of defect engineering for the enhancement of the OL action of graphenes, in view of potential OL applications.

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T14-P: Distinguishing between the Electronic and Thermal Origin Nonlinearities of Single and Few Layered Graphene

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In the present work, the electronic and thermal origin nonlinearities of single-layered (SLG) and few-layered (FLG) graphene dispersions were evaluated and are distinguished using the conventional Z-scan technique and a combination of the Z-scan with thermal lensing technique, under low (i.e., 10 Hz) and high (i.e., 80 MHz) repetition rate laser excitation conditions, respectively.

As shown in Figure 1 (a,b), under low repetition rate laser excitation conditions, SLG and FLG dispersions were found to exhibit saturable absorption (SA, nonlinear absorption coefficient $\beta < 0$) as indicated by the dashed curves obtained, after taking into account the solvent contribution. The observed SA behavior can be explained in terms of the Pauli blocking principle.[1] Concerning the nonlinear refractive response, the SLG sample was found to exhibit a positive nonlinear refractive index parameter γ' , after subtracting the solvent contribution, corresponding to a self-focusing behavior. Figure 1. Open-aperture (a,b) and "divided" (c,d) Z-scans of SLG and FLG dispersions in ODCB and DMF. All measurements correspond to a laser intensity of 1.5 TW/cm^2 . The concentrations of SLG and FLG were 0.06 and 0.1 mg/mL, respectively. Figure 2. Temporal evolution of the CA Z-scans of SLG and FLG dispersed in ODCB and DMF, respectively, obtained experimentally (a,c) and from theoretical calculations (b,d).

It is noteworthy to add that FLG exhibited negligible nonlinear refraction response. From the analysis of the Z-scan data, it was concluded that SLG exhibits a significantly larger third-order susceptibility $\chi(3)$ than that of FLG (i.e., ~ 20 times larger),

attributed to the stronger π -electron delocalization occurring in SLG.[2]

On the contrary, under high repetition rate laser excitation (i.e., 80 MHz), the nonlinear optical response of both SLG and FLG exhibited a dramatic enhancement (see Figure 2), attribute to thermal effects induced by the high repetition rate laser pulses. It must be noted that both solvents did not exhibit any thermal lensing signal for the range of laser power (i.e., 0.7 mW) used for the experiments. Therefore, it was proved that the thermal effects can dominate, under such excitation conditions, obscuring the observation of the electronic origin nonlinear optical response.

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T5-P: Flexible microfluidic chip based on plasmonic paper for efficient MEF detection of immunological reaction

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Efficient and affordable high-throughput plasmonic lab-on-chip (LOC) devices have attracted the attention of scientists in the field of biosensing nanotechnologies as innovative alternatives to the complex, time consuming and expensive conventional diagnostic tools. To overcome these limitations, the

nanotechnology community aims to develop simple, specific, and cheap testing platforms for the rapid and efficient detection of biomarkers. Metal Enhanced Fluorescence (MEF) biosensing devices represent a new detection design relying on the high sensitivity of the MEF phenomenon translated into lower limits of detection and, implicitly, early diagnostic [1]. Moreover, the use of fluorophores with excitation/emission in the Near-Infrared (NIR) region that can easily overlap with the response of the emitter leads to the development of NIR-MEF biosensing devices that -to the best of our knowledge, have not yet been explored in literature. Our work proposes the development of a new innovative, miniaturized, portable and low-cost flexible microfluidic chip based on the integration of plasmonic paper in between two polydimethylsiloxane (PDMS) layers for the efficient and specific detection of the biotin-streptavidin recognition interaction by MEF sensing. Firstly, gold nanobipyramids (AuBPs) were chemically synthesized and further used as plasmonic ink for the fabrication of the plasmonic paper through the calligraphy approach. A fluorescence sandwich immunoassay based on successive injection of human IgG and biotin conjugated human anti-IgG was developed, thus the needed linker for the Alexa680 conjugated streptavidin analyte and, moreover, the necessary metal-to-fluorophore distance for MEF were achieved. Each functionalization step was confirmed by LSPR. Furthermore, by resonantly exciting both AuBPs and fluorophore, the fluorescence emission of Alexa680 was enhanced as the conjugated streptavidin was captured, thus the successful detection of the biotin-streptavidin interaction was indirectly confirmed by MEF. In conclusion, we developed a rapid, low-cost, miniaturized, portable, flexible biosensing chip able to efficiently detect immunological reactions by MEF, hence contributing to the progress of LOC technologies.

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T5-P: Microwave Sensors array for VOC detection and identification

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Volatile organic compounds (VOCs) are ubiquitous environmental pollutants that are emitted as gases from certain solids or liquids. Despite that VOCs are not acutely toxic, some of them may be associated with a long-term adverse health effect, as some have been classified as carcinogenic or probable carcinogens for humans. Concentrations of many VOCs are typically higher indoors than outdoors, so it is very important to develop instruments which can detect, discriminate VOCs and integrate into an environmental control system. Current technologies are far from offering the required sensitivity and selectivity, relying on technologies which are still expensive. We present here the architecture of an array of sensing devices, composed of eight microwave ring oscillators, working in the 60 GHz band (Fig. 1). These oscillators are covered with four customised sensing layers. A decision on the presence of a certain VOC compound

will be taken based on the response of different sensors, part of the array. This will be implemented through a dedicated “sensor data fusion” software module. Further software developments will include the design and implementation of an Artificial Intelligence (AI) module. Our approach brings in 2 technological breakthroughs. The first one relates to the sensing layers; while the starting material (i.e., carbon nanohorns) is commercially available, specific functionalization procedures are considered, to ensure that the customised layer is sensitive to certain chemical and physical features of the VOC molecules. The second breakthrough relates to the design and development of a microwave smart array of sensors, functioning in a frequency band (60 GHz) which has clear advantages: low power for transmission, small size antennas, highly secured communication.

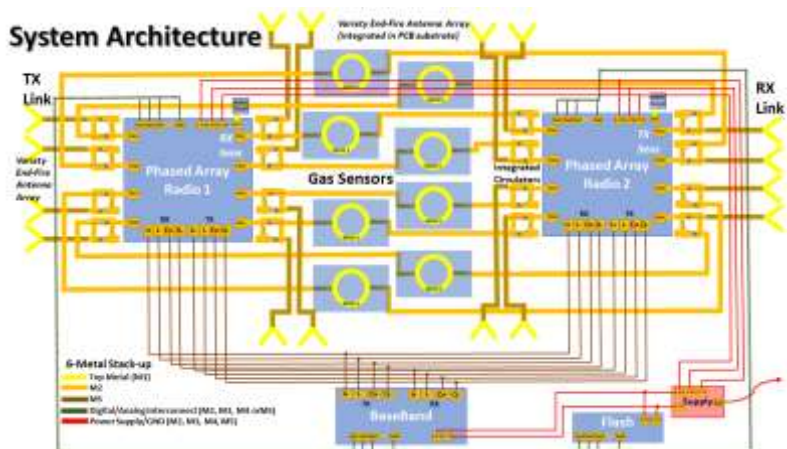


Fig. 1 – GeNOSE system architecture

T4-P: New method for the preparation of amorphous and nanocrystalline powders for magnetic cores applications

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The purpose of our work is to develop, using an improved technique of liquid - gas atomization, powders of composition $\text{Fe}_{73.5}\text{Cu}_1\text{Nb}_3\text{Si}_{13.5}\text{B}_9$ in the amorphous and nanocrystalline state with various dimensions. The improved technique consists in the use of three jets of fluids (two jets of Ar gas and one jet of water), directed in such a configuration so that the molten alloy jet to be successively fragmented in droplets by the two gas jets and further broken into droplets and cooled by the liquid jet. Scanning Electron Microscopy (SEM), X-ray diffraction (XRD), thermomagnetic, and magnetic measurements have been performed to assess the structural and magnetic differences between the groups of samples after sieving. The magnetic measurements have been performed using the Vibrating Sample Magnetometer technique (VSM). The SEM images revealed the formation of particles with almost spherical shape. The structure of particles, with the size of 0-20 μm , 20-32 μm , 32-63 μm , and 63-100 μm have been investigated by X-Ray diffraction and it has been noticed that in the range 0-32 μm there is a mixture of amorphous and nanocrystalline particles with approx. 50 % of particles in amorphous and nanocrystalline state, which is a quite high percentage. This behaviour is due to the difference in the cooling rate of particles. The mixture of amorphous and

nanocrystalline phases was also confirmed by the slope of the thermomagnetic curves, the Curie temperature increasing from 350°C to 520°C. The saturation magnetization of powders takes values between 130 to 145 emu/g, with slight variations. The coercive field, H_c , has the lowest value of 4 Oe for the powders with the smallest diameter range, the value increasing continuously up to 23 Oe for the samples with the larger diameter, for the samples in the as-cast state. Thus, we have obtained powders with a mixture of amorphous and nanocrystalline phase for sizes of up to 48 μm by using an improved atomization technique, which will be used for the fabrication of magnetic cores for high frequency applications. Work supported by the Romanian Ministry of Research, Innovation and Digitalization under NUCLEU Program – contract no. 33N/2019, project PN 19 28 01 01.

T4-P: Phase transition in spin-crossover system with random interaction

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In the regular spin-crossover (SC) lattice, the intermolecular elastic interactions originating from misfit between different molecular volumes for both spin states generates very rich behaviors. The microscopic Ising-like model for SC regular molecular crystals with intermolecular interaction in the fully connected limit is

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} s_i s_j - h \sum_i s_i, \quad (1)$$

where, J_{ij} is coupling between the i -th and j -th spins, $s_{i,j}$ is pseudospin operator with eigenvalues ± 1 . For SC compounds the magnetic field h cannot be zero and is determined as $h = -\frac{1}{2}(\Delta - k_B T \ln g)$. Here, Δ is non-zero crystal field and g is relative degeneracy. We considered the random exchange approach for the interaction J_{ij} in which it can be assumed to have Gaussian distribution:

$$P(J_{ij}) = (2\pi J^2/N)^{-1/2} \exp \left[-N(J_{ij} - J_0/N)^2 / (2J^2) \right]. \quad (2)$$

Within this approach one can see the physical meanings for J_0 and J , that are average value and the standard deviation of intermolecular coupling J_{ij} [1].

To better appreciate the regime without hysteresis, the critical one, and the one with hysteresis we studied numerically the system magnetization m and spin-order parameter q for two opposite cases $J < J_0$ and $J > J_0$ (see, Fig. 1). One can see that the occurrence of a smooth or sudden change of m and q are strongly related to the average intermolecular coupling J_0 . The random distribution of intermolecular bonds destroys the magnetic order in the system.

08:00 **Plenary Session**

HALL 1

10:20 Coffee Break

11:00 **Invited and Oral Session**

HALL 1

13:35 Lunch

15:00 **Plenary Session**

HALL 1

18:00 Coffee Break

18:30 **PLENARY&INVITED & ORAL SESSION**

20:35 Gala Dinner

Hall-1**T10-PL: Towards liquid state cybernetic systems**

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Organic, inorganic or hybrid devices in the liquid state, kept in a fixed volume by surface tension or by a confining membrane that protects them from the environment, could be used as biologically-inspired autonomous cybernetic systems with unique capabilities. A general lack of investigations, approaching at systemic level the development of an amorphous / liquid device, has prevented ever since recognizing the potential of colloidal suspension to trespass conventional systems based on collisional protocols, mass or charge transport and segregated architectures [1]. This innovative solution has been proposed for several future applications, such as space exploration in extreme or otherwise challenging environments, post-disaster search and rescue in ground applications, compliant wearable devices, medical field for in vivo applications, novel computational paradigms [2]. Their subsystems and the enabling nanomaterials will be described, providing mobility [3], energy harvesting / storage [4], sensing of physical stimuli [5], information processing / storage [6], telecommunication capabilities [7].

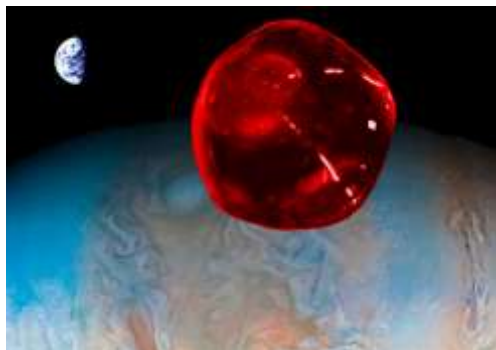


Fig. 1. Pictorial representation of a liquid state autonomous cybernetic system for space exploration. Not in scale are shown: Jupiter clouds (below), the Earth (top left), and the colloidal robot (in red).

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T5-PL: Growth of spinnable CNT and its application to a data glove

281

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²Hamamatsu Carbonics Co., Central Research Laboratories, Hamamatsu, Japan

We have synthesized spinnable carbon nanotube (CNT) [1] and have developed the CNT strain sensors as components of a textile based, wearable sensing system for real-time motion detection [2]. The aligned CNT layer was formed by stacking CNT webs drawn from a spinnable CNT forest. In the strain sensors, we sandwiched the aligned CNT sheet between elastomer layers. We have applied the CNT strain sensors to the data glove as shown in Fig. 1. The data glove detects fine finger motions and collecting electric motion data when worn on the hand.

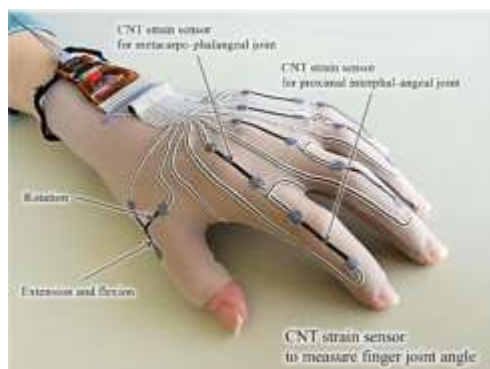


Fig.1 Data glove using the CNT strain sensors.

When a finger joint bends, the respective CNT strain sensor elongates, and the resistance increases. The data glove has generated significant outcomes in various fields that require electric expression of human finger motions, such as virtual

reality (VR) studies, animation and computer graphics (CG) production, and ergonomics. In the presentation. I will introduce the data glove with the CNT strain sensors and the demonstration of the CG, VR etc. using the data glove.

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T7-PL: Epitaxial ferroelectric HfO₂ films

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Ferroelectric HfO₂ is a promising material for new memory devices, but the microstructure of the films needs to be better controlled and some properties such as endurance need to be improved. Research of ferroelectric HfO₂ has been focused mainly on polycrystalline films. In contrast, epitaxial films, of great interest to understand properties and prototyping devices, are scarcely investigated.

The recent stabilization of the orthorhombic ferroelectric phase in epitaxial Hf_{0.5}Zr_{0.5}O₂ films on perovskite substrates [1] has allowed, among other results, to control the crystalline polymorphs through substrate and electrode selection, [2] achieving high polarization, endurance and retention in sub-5 nm films, [3] and the epitaxial integration with Si(001) [4]. Here I will present some of the most relevant findings achieved in our group in the last two years.

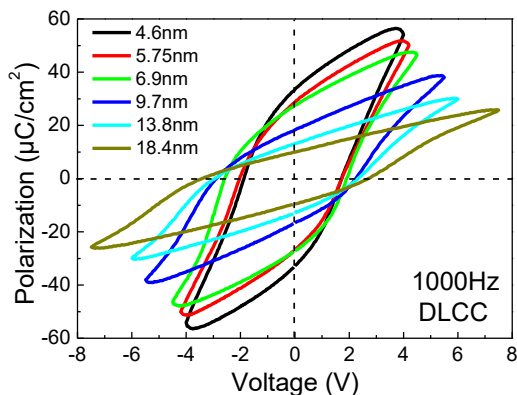


Fig. 1. Ferroelectric polarization loops of epitaxial $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$ films on Si(001). Films thinner than 5 nm show a remanent polarization above $30 \mu\text{C}/\text{cm}^2$.

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T11-PL: Nanoscale effects in strained epitaxial films: when elasticity and capillarity dynamically compete

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The development of new semi-conductor technology involves strain engineering as a powerful tool to modulate electronic properties such as band structure, mobility .., e.g. in the Si and SiGe layers of gate and source/drain areas. Alternatively, strain may be used to drive the morphological evolution during

growth or annealing of nanofilms, e.g. in strained SiGe layers on Si(001) that eventually lead to self-organized nanostructures such as quantum dots. In both cases, the knowledge of the coupling between elastic effects and of capillarity is crucial to control the epitaxial systems [1]. Using different examples, we will review the theoretical knowledge of the surface dynamics related to strain at the nanoscale. We will analyse the development of the Asaro-Tiller-Grinfeld (ATG) instability and its dynamical competition with the usual nucleation at work when strain is strong enough [2]. We will also show how strain may enforce a counter-intuitive attraction between nucleated quantum dots [3]. Eventually, we will also report a new morphological evolution of a strained epitaxial film deposited on a mesa driven by strain inhomogeneity due to finite-size effects [4]. Unlike the ATG instability originating from the relaxation due to surface corrugation, this evolution arises due to the static inhomogeneity originating from free frontiers.

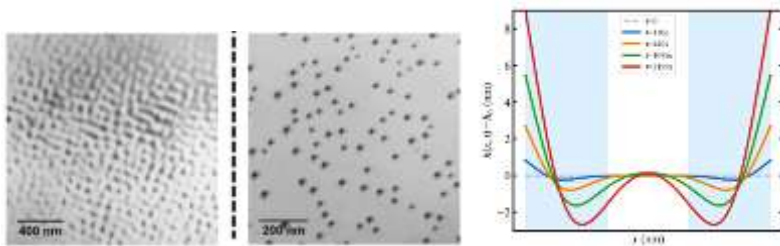


Fig. 1. (Left) TEM images of SiGe films deposited on Si(001) with a mean Ge composition of 0.3 (left) and 1 (right) ; (Right) Theoretical evolution of a strained mesa near its free boundaries.

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- [4] K. R. Hannikainen, L. Favre, A. Ronda, I. Berbezier, D. Dutartre, J.-N Aqua, *to be published*.

INVITED AND ORAL SESSIONS

HALL 1

T6-I: The role of adsorbed ions (adions) at metal molecule interface in plasmonic nanoparticles

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Plasmonic nanoparticles (NPs) are promising materials due to their ability to collect light in the visible range and due to localized electromagnetic field enhancements. The light harvesting ability makes them of interest for a variety of technologies that rely on the conversion of photons into energetic charge carriers (*e.g.*, photovoltaics, photocatalysis), whereas the enhanced electromagnetic field in the vicinity of the NP is exploited in optical sensing methods such as surface-enhanced fluorescence or surface-enhanced Raman scattering (SERS).

The adsorption of molecules to the metal nano-surface is required for both chemical reactions at the nanoparticle surface, and surface-enhanced optical methods, due to the rapid intensity decay with distance of the electromagnetic field.

However, our physicochemical understanding of the metal–molecule interface is still in its early stage.

In our research, we highlight the role of adsorbed atomic ions (adions) in SERS, which give rise to a surface effect, which enables the selective adsorption of anionic and cationic analytes. According to our proposed adion specific adsorption model, cationic adions such as Ag^+ , Ca^{2+} , Mg^{2+} , Al^{3+} , promote the chemisorption of anionic species, as shown for Cl^- and several organic acids, and in turn, anionic adions such as Cl^- , Br^- , I^- promote the chemisorption of cationic molecules, as shown for several cationic dyes [1]. Based on this finding, we show the selective SERS detection in real life applications such as the selective SERS detection of purine metabolites and proteins in the complex matrix of urine biofluid. Moreover, we validated the adion specific adsorption model even at single molecule level [2].

The adsorption of halide ions to the metal surface is of particular interest, due to their ability of partially charging the metal NP, raising thus the Fermi energy of the NP. We highlight two effects as consequence of the increased reactivity of the NP. Firstly, we show a faster dissolution of Ag NPs when supplementing the colloidal solution with I^- . Moreover, we use a remarkably simple method to increase the chemisorption rate of I^- by generating additional adsorption active sites via Mg^{2+} adions and consequently further increase the dissolution rate of metallic Ag NPs.

Secondly, we highlight a new metal-molecule charge transfer process by tuning the Fermi energy of plasmonic Ag NPs in situ. The strong adsorption of halide ions upshifts the Fermi level of

Ag NPs by up to ~ 0.3 eV in the order $\text{Cl}^- < \text{Br}^- < \text{I}^-$, favoring the spontaneous charge transfer to aligned molecular acceptor orbitals (Fig. 1) until charge neutrality across the interface is achieved [3].

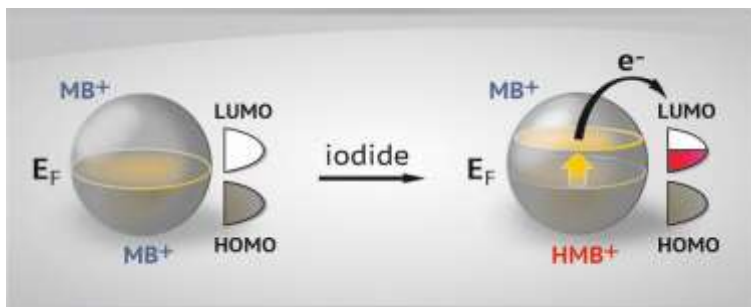


Fig. 1. Schematic illustration of Fermi energy increase after I^- adsorption and alignment with the acceptor state of methylene blue (MB^+). In consequence, an electron is transferred into the acceptor state, reducing MB^+ to HMB^+ .

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T8-I: Chemically designed silicones for 3D printing technology

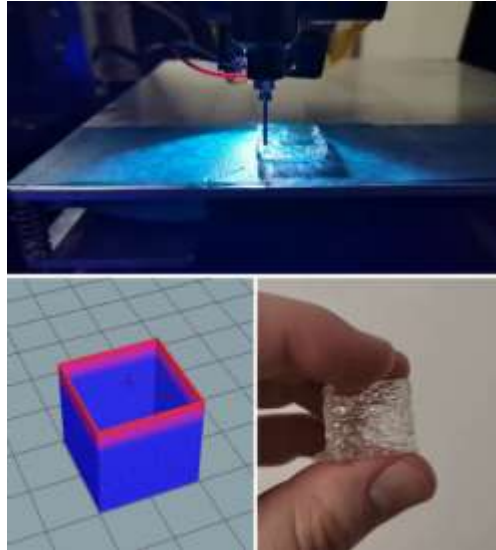
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Silicone rubbers are some of the most widely used for dielectric elastomer transducers (DETs) technology.[1] Current DET manufacturing technologies are based on spin-coating and spray coating processing.[2] However, for the prototyping of small series of customized products, this process may be expensive.[3] This has motivated the development of 3D printing technologies, which allows the construction of three-dimensional objects following a digital model. Because silicone materials such as thermosetting polymers cannot be thermally processed, a completely different printing process is required. There are few groups of researchers working on silicone 3D printing technologies.[4] Unlike such technologies, our printing process for full silicone formulations based on UV-activated thiol-ene addition of α,ω -bis(trimethylsiloxy)poly(dimethylsiloxane-co-thiopropylmethylsiloxane) to α,ω -bis(trimethylsiloxy)poly(dimethylsiloxane-co-vinylmethylsiloxane) is considered "green" since it requires low energy consumption and is free of solvents and metal catalysts.



The silicone formulation developed allows the deposition of smooth and uniform layers with a resolution of up to 200 μm , as well as rapid printing process. Moreover, the variation of molecular weight and crosslinking density enables tunability of mechanical strength, elasticity, stretchability, and electromechanical response. Mechanical tests revealed that the printed elastomers are capable of undergoing hundreds of cyclic deformations at 100% strain without visible hysteresis. Similarly, the electromechanical tests show a substantial change in actuation strain and dielectric strength through variation of the two structural parameters. Along side the customized-formulated silicones, the new built 3D-printing machine with adaptive mechanical and software parameters allow its users to create highly complex-shaped objects and may serve as a springboard for new directions in DET technologies and beyond.

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[2] F. Mashambanhaka, Silicone 3D Printer – All You Need to Know in 2019

[3] S. J. Grunewald, WACKER Announces New Silicone 3D Printing Technology, 2015.

T8-O: Polyimides containing bipyridyl-amine functionalized triphenylamine as electrochromic materials

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Electrochromic (EC) materials have attracted the researcher's interest owing to the wide range applications in various fields, including optical storage, automotive rearview mirrors, smart windows in buildings, displays and electronic paper. For practical use, EC materials must obey some characteristics, such as rapid response time, high color contrast, excellent cycle life and low driving voltage. From this point of view organic polymers, including polyimides are among the most promising EC materials due to their diverse color variation and long service life as compared to the inorganic and small molecule materials [1]. Polyimides (PIs) possess outstanding mechanical, electrical and radiation resistance properties, which evolve from the strong intramolecular and intermolecular charge transfer interactions. Thus, PIs have poor solubility and processability, which limit their widespread use and many efforts have been undertaken to overcome these limitations, like incorporation of bulky electroactive triphenylamine (TPA) units. Aromatic PIs bearing TPA units show interesting redox-active and electrochromic behaviors in addition to their inherent properties, such as high thermal stability. TPA can undergo easy oxidation reactions to form radical cations having

good stability, which is frequently associated with a strong change in color. A series of TPA-based PIs with excellent physical properties including good solubility, high thermostability and electrochromic performances have been already developed in our lab [2,3]. In the frame of these perspectives, here we present the synthesis and characterization of a series of polyimides incorporating bipyridyl-amine functionalized triphenylamine and various flexible linkages with focus on physico-chemical properties and electrochromic behavior.

Acknowledgements: This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, Project PN-III-P2-2.1-PED-2019-3520, 438PED/2020, within PNCDI III.

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T8-O: Dielectric Spectroscopy Investigation of Novel Hybrid Composites Obtained From Cellulose Derivatives Doped with 1-Hydroxybenzotriazole

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There is no doubt that our civilization is embracing technology like never before. As the global smart home market evolves, many new devices will be developed, requiring alternative power sources. Recently, a major concern has been for development of miniature fuel cells for portable electronic devices. Among various categories of fuel cells, the polymer electrolyte membrane fuel cells (PEMs) are highly distinguished due to their practical performances, such as easy fabrication, low costs, good mechanical properties, chemically inert, etc. The microcrystalline cellulose doped with heterocycles-type materials may be employed as alternative membranes mainly due to high proton conductivity, good swelling properties, and improved mechanical properties of heterocyclic molecules. Here, we present dielectric spectroscopy investigations of some hybrid composites with respect to their proton conductivity properties. Three type of cellulosic support, such as cellulose acetate (CA), cellulose (C) and oxidized cellulose (Cox) were employed as matrix. As doping agent we opted for 1-Hydroxybenzotriazole (HBT) being known its ability to conduct protons. The proton conductivity values were evaluated from the typical Cole-Cole plots. The impact of HBT on the proton conductivity properties of hybrid composites was evaluated by varying the dopant loading between 10-50 % wt. We show that the hybrid membranes reveal good proton conductivity in a broad range of temperature. The activation energy of membranes will be evaluated and discussed in order to determine the best polymer matrix that favors the transport of charge carriers.

Acknowledgements: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE-2020-0476, within PNCDI III.

T8-O: Surface functionalization of inorganic nanoparticles for covalent immobilization in polymer matrices

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Nanotechnology has experienced a fast development due to the variety of potential applications (industrial and military) that have attracted investments of billions of dollars in this research field. Over the last years, nanotechnology has gained a prominent role in our daily life, in 2014 being available over 1800 consumer products containing nanomaterials in their composition (e.g. paints, coatings, catalysts, cosmetics, some food products, food packaging, clothing, disinfectants, electronics). Related to this topic, intensive studies were focused on the synthesis of hybrid materials, constituted of both inorganic and organic elements, since the resulting hybrid composites have proved to display superior mechanical, thermal, optical or electrical properties [1]. Up to now, an extensive collection of polymer nanocomposites achieved by combining different inorganic components (metals, metal oxides, clays or silica) with various polymer host have been developed, emphasizing the benefits of the synergic features on the properties of the resulting composites. However, a major concern related to the preparation of hybrid nanocomposites consists in the inherent immiscibility between the inorganic and organic phases, reason for that many research efforts were directed toward the chemical modification of inorganic nanoparticles in order to increase phase compatibility, promoting an enhancement of matrix-nanoparticle interactions. The most common coupling agents are silane derivatives, a type of compounds that may act as molecular bridges able to favour the interfacial adhesion

between the inorganic fillers and the organic phase [1,2]. Our group also works on surface functionalization of inorganic nanoparticles (TiO₂, CeO₂) for their covalent immobilization and dispersion in the polymer matrices (polyurethane, cellulose). The resulted hybrid materials are deeply characterized in order to assess their potential application (UV shielding, photocatalysis s.o.).

Acknowledgements. This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-TE-2019-1245 (23/27.08.2020), within PNCDI III.

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T8-O Cellulose-derived platforms for targeted technological applications

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Cellulose has been used for always for rudimentary purposes, for basic human needs (e.g. building material, energy producer and paper manufacturing material), but in modern era, cellulose has acquired new dimensions of knowledge and scientific interest and becomes a valuable resource providing derivatives with a high degree of built-in technology that have unpredictable applications. Also, cellulose represents an unlimited source of versatile raw materials for the increasing demand of environmentally friendly, sustainable and biocompatible products [1]. Cellulose and its derivatives with their unique chemical structure have been found to be versatile materials that provide a high-quality platform for carrying out

the immobilization process of inorganic nanoparticles, biomolecules s.o. Despite all these advantages, its main issues are the poor solubility and processability. To solve these problematic matters, cellulose acetate (a cellulose derivative) is often used as starting support for specific immobilization, because it's excellent solubility in organic solvents, and remarkable film forming properties. The use of cellulose acetate ensure a high versatility of the overall system, since cellulose structure can be regenerate on the surface, through deacetylation reaction [2], and even by further selective oxidation process is provides oxidized cellulose bearing carboxyl moieties [3]. In view of all these information, this study reports the fabrication of a tuneable and flexible reproducible cellulose-based platform for immobilization of inorganic nanoparticles with tailored properties through surface modification of cellulose host for directed applications. Acknowledgements: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P2-2.1-PED-2019-0169, within PNCDI III

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T10-O: High thermal conductivity nanocomposites with two-dimensional materials for thermal load management in shape memory alloy devices

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Shape memory alloys are modern multifunctional materials with controllable shape, with possible uses for the actuation in various applications. One of the most important challenges after the martensitic phase transformation actuation in shape memory alloys consists in lowering the temperature of the composite. Boron nitride (BN) nano-objects with defined shapes such as rods and 2D sheets possess high thermal conductivity [1,2] and nanocomposite materials with 2D BN nanosheets provide an excellent alternative to graphene nanocomposites for high thermal conductivity materials with rapid dissipation of thermal load and lowering the temperature of the object [3]. We encapsulated active elements of Ni-Ti-Cu shape memory alloy with controlled size and shape into polymer nanocomposite with 2D BN nanosheets and we demonstrated the capability of such nanocomposites to transfer significant amounts of heat by conductivity. The BN sheets were exfoliated using a well-known method [3]. The exfoliated 2D BN nanosheets were mixed in a dual asymmetric

centrifugal mixer with a silicone matrix polymer and the material was used by room temperature condensation for encapsulation of Ni-Ti-Cu shape memory alloy. The nanocomposites thus prepared bring together in a synergistic manner the capability to store elastic energy specific to silicone elastomers and the excellent thermal conductivity and film forming ability specific for 2D BN nanosheets. Thus, the nanocomposites have thermal conductivities >50 W/mK, close to the values for aluminium alloys. This in turn allows decrease of active element temperature from >40 °C to less than 20 °C in under one minute. The elastic energy is stored in the silicone elastomer and the cooling of the shape memory alloy allows these to reverse to initial state with excellent repeatability (>1000 cycles).

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T10-O: Preparation and Properties of p(N-Isopropylacrylamide-co-butylacrylate) Coatings using Matrix Assisted Pulsed Laser Evaporation method

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Matrix-Assisted Pulsed Laser Evaporation (MAPLE) method was used to obtain Poly (N-isopropylacrylamide-co-butylacrylate) (pNIPAM-co-BA) functional and thermoresponsive coatings. The influence of the laser fluence and various solvents on the morphological and chemical characteristics of the coatings were evaluated. For example, the morphology, roughness and hydrophobic/hydrophilic character, as well as the thermoresponsive capacity were investigated by atomic force microscopy and contact angle measurements. The chemical characteristics of the pNIPAM-co-BA coatings were analysed by Fourier Transform Infrared Spectroscopy (FTIR) and XPS. The chemical functionality was retained in all samples obtained with MAPLE and the thermoresponse was demonstrated by the change in the contact angle and thickness values when the temperature was shifted from 37 °C to 24 °C.

T10-O Structural studies on some dental composites containing polyglass and gold nanoparticles as aditives

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We present our results obtained by analyzing nanocomposite cements developed by mixing zinc polycarboxylate with polyacrylic acid and 11%wt polyglasses or/and hydroxyapatite and 5%wt gold nanoparticles. The synthesis and characterization of amorphous polyglass powder, hydroxyapatite and gold nanoparticles is presented together with the structural and functional properties of nanocomposites.

Compared to the zinc polycarboxylate cement the composites obtained by adding polyglasses and/or hydroxyapatite and functionalized AuNPs are more homogeneous. Functionalized AuNPs increase the matrix porosity, the so obtained nanocomposites being favorable for applications as dental cements or as scaffolds for bone growth. The AuNPs irradiation with green light increases the reactivity with the polyacrylic acid and the pore sizes.

Online

T14-I: Hollow core optical fibers for nonlinear microendoscopy

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We review our recent work about negative curvature hollow core optical fibers optimized for nonlinear microendoscopy. The fiber design (shown in Fig. 1) allows distortion-less, background-free delivery of femtosecond and picosecond excitation pulses over a >1000 nm spectral range, and the back-collection of nonlinear signals through the same fiber. Sub-micron spatial resolution together with large field of view is made possible by the combination of a miniature objective lens together with a fonctionnalization of the fiber output (silica microsphere lens inserted into the fiber core or GRIN fiber spliced to the output facet).

With these technologies, we present a flexible, compact, and multimodal nonlinear endoscope (2.2 mm outer diameter). We demonstrate coherent anti-Stokes Raman scattering, 2-photon fluorescence and second harmonic generation imaging at a rate of 10 frames/s. The route towards 3-photon fluorescence and third harmonic generation will be explored.

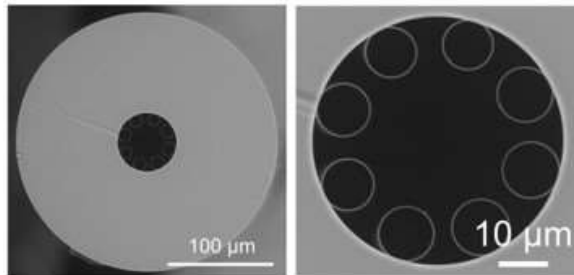


Fig. 1a - Scanning electron microscope image of the negative curvature hollow core fibre developed for nonlinear endoscopy

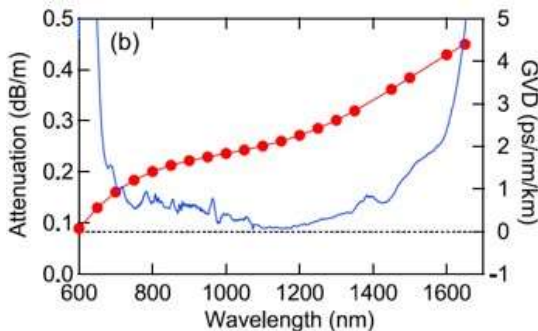


Fig. 1b - Attenuation spectrum (blue line) and measured group velocity dispersion (red markers) of the fiber.

T14-I: From GeSi to SiGeSn alloy nanocrystals with benefits in SWIR detection

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Here we present our latest results related to development and engineering of advanced nanomaterials and nanostructures with applications in optoelectronics and photonics, based on group IV Si-Ge-Sn semiconductor nanocrystals (NCs) embedded

in oxides (SiO_2 , TiO_2 , HfO_2) [1–4]. Development of devices based on group IV elements, with high sensitivity from VIS to NIR and SWIR is a hot topic within the effort to achieve monolithical integration for chip-scale Si photonics, i.e. LED-Photodetector-Laser trinity.

We achieve materials fabrication by the cost-effective, versatile and ecologic magnetron sputtering deposition followed by *in situ* nanostructuring during growth and/or *ex situ* rapid thermal annealing.

We will show different concepts and strategies for engineering group IV NCs morphology (density, composition, size, surface passivation) and bandgap and increasing their thermal stability.

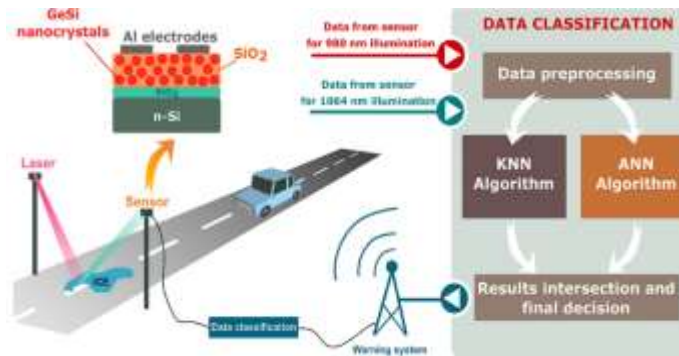


Fig. 1. Working principle of GeSi NCs-based sensor setup for detection of road conditions: asphalt is illuminated sequentially with 980 and 1064 nm laser diodes; photoresponse (photocurrent) of sensor under illumination with light reflected from asphalt having different reflection coefficients for dry, wet, icy and dirty ice coatings is measured; database of photocurrents is obtained for different road conditions; k-nearest neighbor and artificial neural networks classification algorithms are used together for accurate recognition of the class corresponding to a specific road state [1]

By obtaining Ge-rich GeSi NCs much more thermodynamically stable than Ge NCs (hindering Ge fast diffusion), much stronger quantum confinement effect in GeSi NCs than Si NCs is ensured, and by choosing proper oxide, optimal separation between NCs and high NCs density is accomplished. GeSi NCs are thermodynamically stabilized by protective SiO₂ layers formed by RTA at GeSi/oxide interface in multilayers or at NC surface in films. Other viable solution is using a high-k oxide matrix such as HfO₂ ensuring better diffusion barrier and low defects density related to good NCs surface passivation. Materials are further engineered by preparing alloy SiGeSn NCs with high benefits from alloying with Sn by SWIR decreased bandgap. Materials engineering is oriented function of application, either for obtaining high responsivity in targeted spectral window or for obtaining sensitivity in wide spectral domain. So, we fabricated different photonics and sensing devices, e.g. optical sensors using GeSi NCs embedded in SiO₂ matrix that discriminate between different slippery road conditions (wet and icy asphalt and asphalt covered with dirty ice) in respect to dry asphalt (working principle in Fig. 1) for assessing traffic safety [1, 5].

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T14-O: Metasurface structures for electromagnetic field enhancement

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This paper presents several metasurface used to enhance the electromagnetic field in order to improve fluorescent emissions in VIS and NIR with possible for biosensing applications. The fluorescence (FL) of a molecule depends on the environment due to the Purcell effect [1]. A method to shape the electromagnetic field for enhancing the FL is based on metasurfaces composed of different shapes and sizes of metallic nanostructures. Fluorescent and light-emitting metasurfaces are obtained by covering the metasurfaces with layers containing quantum dots, dye molecules, nanoparticles, or by integrating direct bandgap semiconductors into the metasurface [2].

We achived promising results analyzing metasurfaces based on ultra-thin metallic films and an active layer containing fluorophore (Rhodamine 6G) dispersed in a PMMA matrix that increases the FL intensity deposited on different substrates (dielectric or semiconductor), We obtained random shapes nanostructure by depositing, on a glass or silicon (Si) substrate, a thin aluminum (Al) film which basically is discontinued, being composed of nano-islands. In fig.1 one can see a SEM image of two such films (Fig.1a–2nm thickness, Fig.1b–4nm thickness).

To analyze the fluorescent intensity for these types of structures we deposited on these nanostructured Al layers (Al NS) solutions of Rhodamine 6G (R6G) dispersed in PMMA in three concentrations ($C_1=50\mu\text{M}$, $C_2=10\mu\text{M}$, $C_3=5\mu\text{M}$) (see table 1). The measurements were performed using FLS920 Fluorescence Spectrometer with $\lambda_{\text{excitation}}=480\text{nm}$ and $\lambda_{\text{emission}}=548\text{nm}$. In table 1 are illustrated the most significant results obtained on the 2 nm film with R6G in PMMA.

One can see that the best intensity is achieved using the highest concentrations C_1 in the thinnest PMMA layer (deposited at 6000rpm). It is important to notice that for the PMMA layers doped with R6G deposited on plain Si the intensity's maximum value is 2900 a.u. (sample 7), whereas in the case of the layers of deposited on substrates covered with the metasurface composed of Al NS the value of fluorescent intensity increases up to 82000 a.u. In conclusion, we showed that the presence of a metasurface composed of random shape Al NS can increase the FL up to 28 times.

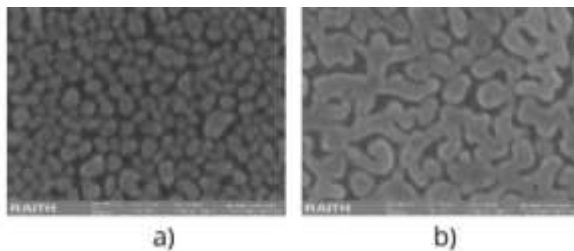


Fig. 1 SEM image of Al film deposited by electron-beam deposition: a) 2 nm thickness; b) 4 nm thickness

Table 1. Fluorescent intensity function on concentration and deposition rate

Sample	Substrate	Concentration R6G in PMMA	Deposition conditions	Intensity (a. u.)
1.	Al NS/Glass	C1	6000 rpm/40 s	176 000
2.	Al NS/Glass	C3	3000 rpm/40 s	110 000
3.	Al NS/Glass	C3	6000 rpm/40 s	95 000
4.	Al NS/Silicon	C1	6000 rpm/40 s	82 000
5.	Al NS/Silicon	C3	3000 rpm/40 s	52 000
6.	Al NS/ Silicon	C3	6000 rpm/40 s	12 000
7.	Silicon	C1	6000 rpm/40 s	2900

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T10-O: Structural changes induced by neutron irradiation of gadolinium doped borosilicate glasses

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The resulting high neutron radiation dose specific to nuclear reactors contributes to the ageing of auxiliary components used to study the experimental outcome of nuclear interactions. Some nuclear reactors use collimated high flux

neutron sources to investigate nuclear reactions for in depth structural analysis by neutron scattering experiments. A key component of such an experimental setup is represented by neutron guides, which are supermirrors used to transport neutrons over great distances with a minimum loss in intensity. These supermirrors are made of multiple layers of borosilicate glass usually coated with a $^{58}\text{Ni}/\text{Ti}$ multilayer. Since a guide has to transport a single pulse, a flux of $10^{11} \text{ n cm}^{-2} \text{ s}^{-1}$, multiple absorption reactions in ^{10}B are produced, which induce a high degradation effect of the glass substrate over time. In order to quantify the type of damage induced by thermal neutrons on gadolinium doped boro-silicate glasses, compositional and structural analysis were performed before and after irradiation to observe the induced changes. The scanning electron microscopy images showed crystallization centers of the glass before irradiation and their distribution in glass. Raman and electron paramagnetic resonance spectroscopy detected the apparition of defects in glass after the irradiation. Crystalline phases were identified using X-ray diffraction technique. Thermal dilatometry measurements were performed to study the best thermal resistant glass composition under the neutron irradiation. Elemental analysis was performed using X-ray photoelectron spectroscopy to observe possible losses of some elements. The observed results on the studied vitreous network compositions of glasses with different gadolinium concentrations suggest the possibility of incorporation of gadolinium in neutron guide systems due to the lower induced amount of defects.

T10-O Downscaling to the critical dimension for stability of the ferroelectric phase in BST ceramics

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Fundamental problems of ferroelectricity that are not yet fully elucidated can be answered by reducing the grains size in ferroelectric materials to the nanoscale level. This method also brings some challenges, with grain boundary and interface density increasing as much as the defects related to chemical heterogeneity. The scale-based phenomena make a general contribution to macroscopic properties and can induce new ones. To find the critical dimension that still facilitates the existence of ferroelectricity at room temperature, dense and fine-grained $\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$ (BST, $x=0.2$ and 0.4) ceramics were sintered from ultrafine BST nano-powders (average particle size estimated at ~ 55 nm) processed via sol-gel method. The two compositions are in different phase states at room temperature, $\text{Ba}_{0.8}\text{Sr}_{0.2}\text{TiO}_3$ is in the ferroelectric tetragonal state, while $\text{Ba}_{0.6}\text{Sr}_{0.4}\text{TiO}_3$ is in the paraelectric cubic state without spontaneous polarization. Structural, microstructural, and dielectric properties were investigated to clarify the effects of the nanoscale chemical heterogeneity, grain size, and boundary/interfaces-related phenomena on the functional properties.

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T10-O: Structural characterization of rare-earths doped TiO₂ nanofibers

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La³⁺, Sm³⁺ and Er³⁺ doped TiO₂ semiconductor nanofibers were fabricated by electrospinning-calcination method and thoroughly characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy and mapping (EDX) and X-ray diffraction (XRD) in order to understand the dopant effects on material structuring compared to pure TiO₂ electrospun nanofibers. Detailed structural characterization shows that the nanofibers have a polycrystalline structure, the crystallites size depends on the type of RE dopant and the dopants have a uniform and homogeneous distribution in the nanofibers. XRD characterization confirmed the presence of the anatase phase in the nanofibers, as the electron microscopy observations did. Nanostructuring plays a deterministic role for their electronic and optical properties. The present study provides essential information for a further understanding of nanofibers functionality in applications such as photocatalysis and optoelectronics.

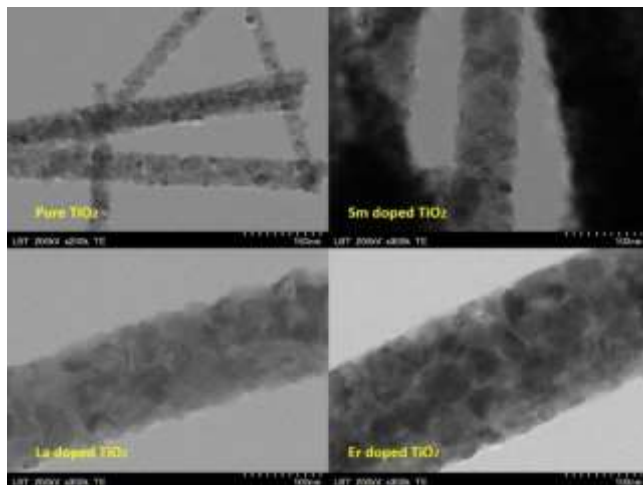


Fig. 1. The image shows TEM images of pure TiO_2 and La^{3+} , Sm^{3+} and Er^{3+} doped TiO_2 semiconductor nanofibers.

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Online

T6-PL: Tip-enhanced spectroscopies on 2-dimensional transition metal dichalcogenides and their interfaces

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Two-dimensional (2D) semiconductors are one of the most extensively studied materials showing potential in a large spectrum of applications from electronics/optoelectronics to photocatalysis and CO₂ reduction. These materials possess astonishing optical, electronic, and mechanical properties, which are different from their bulk counterparts. Due to strong dielectric screening, local heterogeneities such as edges, grain boundaries, defects, strain, doping, and chemical bonding dictate their physical properties to a great extent. Therefore, there is a growing demand of probing such heterogeneities and their effects on the physical properties of 2D semiconductors on site in a label-free and non-destructive way. Tip-enhanced Raman spectroscopy (TERS), which combines the merits of both scanning probe microscopy and Raman spectroscopy, has experienced tremendous progress since its introduction in the early 2000s and is capable of local spectroscopic investigation with nanometer spatial resolution (Fig.1). Introducing this technique to 2D semiconductors not only enables us to understand the effects of local heterogeneities, it can also

provide new insights opening the door for novel quantum mechanical applications.

In this contribution we deliver a short introduction to the most commonly used 2D semiconductors, namely the transition metal dichalcogenides (TMDs), and their properties. Subsequently we briefly introduce the basics of TERS as well as tip-enhanced photoluminescence (TEPL). Then we discuss several examples highlighting the application of tip-enhanced optical spectroscopies (TEOS) to 2D semiconductors.

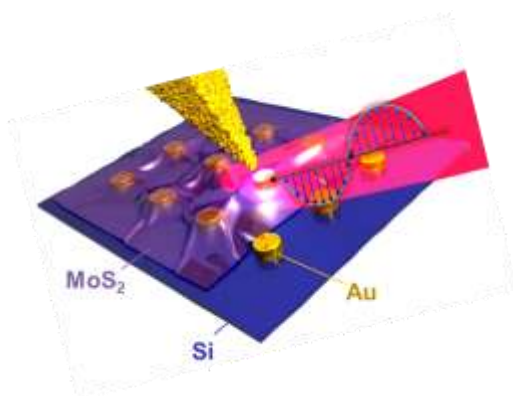


Fig. 1. Sketch of a TERS experiment investigating a MoS_2 monolayer deposited on an array of gold nanodisks on silicon. The gold tip of an atomic force microscope is tilted and the laser light focused onto the tip apex is polarized along the long tip axis for strong coupling to the localized surface plasmon resonance. The scattered light is collected by the same lens focusing the laser onto the tip.

T4-PL: Multiscale analysis of perpendicular magnetic anisotropy and its electric field manipulation in spintronic devices

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The electric field manipulation of magnetization [1,2] represents today a major paradigm in the new generation spintronic storage devices since it provides extremely low energy consumption and sub-nanosecond switching time. The yield of such process depends on the anisotropy energy variation in response to the applied electric field and therefore a wide variety of studies have been dedicated to this topic.

In this work we present a combined experimental-theoretical study of the perpendicular magnetic anisotropy (PMA) electric field modulation. Moreover, we illustrate the Rashba origin of the Dzyaloshinskii-Moriya interaction (DMI) and the possibility to control its sign and amplitude by tailoring the multilayer stack sequence. The ab-initio calculations of voltage-controlled PMA have been performed using the Full Potential Linear Augmented Plane Wave FP-LAPW *Wien2k* code [3]. Based on the anisotropy and DMI data extracted from the DFT calculation, we performed micromagnetic simulations combined with artificial intelligence (AI) analysis algorithms to derive complete phase diagrams of magnetic configurations. From these, we extract the magnetic parameter range in which one could stabilize skyrmionics chiral structures and illustrate how these could be further manipulated by electric field sequences (see Fig.1), as requested in storage or artificial synaptic devices.

Au/Fe/MgO $M_{\text{sat}} = 1400 \cdot 10^3 \text{ A/m}$; $A_{\text{ex}} = 3.0 \cdot 10^{-11} \text{ J/m}$ - Fe exchange stiffness, $\alpha = 0.5$, $256 \times 256 \text{ nm}$, 1 nm thickness

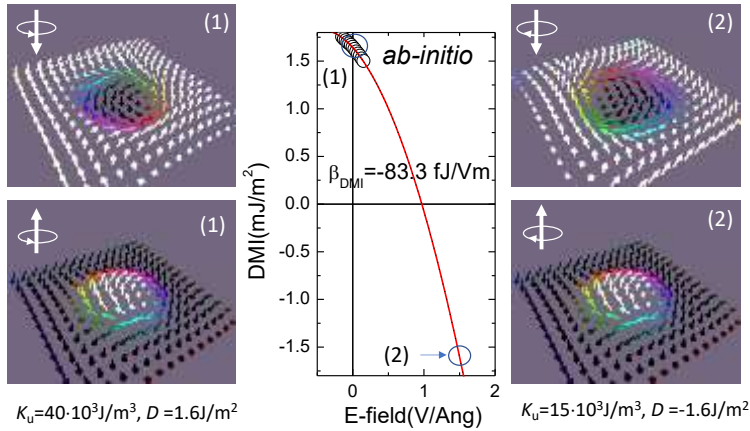


Fig.1 Calculation of DMI dependence of electric field in Au/Fe/MgO(001) supercell. The gate controlled 4 state skyrmionic system: 2 chiralities + 2 core orientations) simulated by the mumax3 micromagnetic code [4].

The theoretical predictions have been used to grow by sputtering samples and pattern spintronic devices dedicated for the experimental analysis of the voltage response of magnetic anisotropy. In these devices, supplementary insight into the anatomy of the mechanisms involved in the electric field effect on the coercive field, driven by the electric field modulation of the surface anisotropy, is further provided within the framework of the LLG macrospin approach.

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Over the last three quarters of the century, since Magnetic Resonance phenomena was first time described and experimental measured, a large number of methods have been developed, growing in today's multi billions market. The techniques have evolved from laboratory demo setups to powerful instruments/tools of our days for addressing numerous physical, chemical and biological problems across various disciplines.

Material science is one of the areas that has taken the advantage, since MR capabilities provides molecular level structural and dynamics information, regardless of the system is solid, liquid, or gaseous state.

Magic Angle Spinning (MAS) technique is the most widespread Nuclear Magnetic Resonance (NMR) methods and is the only one, that allows high resolution NMR spectrum, acquired on solids, semi-solids, or a mixture thereof [1].

Tunable pressure and temperature (TPT) magic angle spinning (MAS) NMR capability [2, 3] have been recently developed to further enhance techniques capability. In order to strike the sensitivity drawback issue, a further step development has been taken when polarization transfer compatibility was developed [4].

[1] R.V.F. Turcu, D.W. Hoyt, K.M Rosso, J.A. Sears, J.S. Loring, A.R. Felmy, J.Z. Hu, J. Magn. Reson. 226 (2013) 64 – 69.

[2] D.W. Hoyt, J.A. Sears, R.V.F. Turcu, K.M. Rosso and J.Z. Hu; US PTO, Patent Number: US 8,692,548 B2, 2014.

[3] D.W. Hoyt, J.A. Sears, R.V.F. Turcu, K.M. Rosso and J.Z. Hu; US PTO, Patent Number: US 9,835,698 B2, 2017.

[4] R.V.F. Turcu, S. Simon; US Patent and Trademarks Office, Patent (Pending) No: 14/457,919, 2014.

T1-PL: 2D materials in field-effect electronic devices

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Two-dimensional (2D) materials are promising candidates for electronic, optoelectronic, and sensing devices.

In this talk, several applications of 2D materials in transistors, sensors, and field-emitters are reported. The focus is on the wide family of transition-metal dichalcogenides (TMDs), such as MoS₂, WSe₂, PdSe₂, and PtSe₂. Nanosheets of TMDs, obtained by either mechanical exfoliation or chemical vapor deposition on SiO₂/Si substrates, are used to discuss electric transport, modulation of the conductivity by a back-gate, photoresponse, effect of electron irradiation, and the role of surface adsorbates.

It is shown that light causes photoconductive and photogating effects as well as desorption of adsorbates, which might result in both positive and negative photoconductivity. It is highlighted how the two types of photoconductivity can coexist in the same device, the dominance of one over the other being controlled by the environmental pressure (Fig.1). Electron

irradiation strongly affects the performance of the devices and is exploited to reduce the Schottky barrier at the contacts, thus improving the TMD/metal contacts. It is shown that adsorbates can change the polarity of the charge-carriers and enhance the hysteresis in the transfer characteristics of TMD-based field-effect transistors.

The dominant n-type behavior in a high vacuum and the sharp-edge geometry, as well as the presence of defects, facilitate the extraction of electrons (field emission) from 2D materials upon application of an electric field. It is demonstrated that TMDs are effective field-emitters and that their emission current can be modulated by a gate.

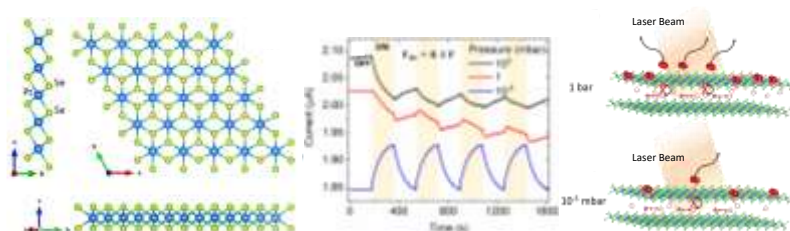


Fig. 1. (a) PtSe₂ structure. (b) Current in a PtSe₂ transistor at different pressures and under laser pulses, showing the coexistence of positive and negative photoconductivity. (c) Light-induced oxygen desorption in PtSe₂.

- [1] A. Grillo et al. *Adv Func Mater* (2021) 2105722.
- [2] F. Urban et al. *Appl Phys Lett* 117 (2020) 193102.
- [3] A. Pelella et al. *ACS Appl Mater Interfaces* 12 (2020) 4053.
- [4] A. Di Bartolomeo et al., *Nanotechnology* 31 (2020) 375204.
- [5] A. Di Bartolomeo et al., *Adv Electron Mater* 6 (2020) 2000094.

T10-PL: New results on photoinduced nanocomposites

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We consider new trends in the field of photo/laser induced growth of inorganic nanoparticles within polymer matrices and examine further developments of the theoretical models, laser-induced growth of core-shell nanoparticles and employment of elaborated matrices. We report laser-induced luminescent micro-structures formed both by direct writing and by means of the mask of colloidal microparticles (Fig. 1). The possibility to enhance the contrast of the laser-recorded structure by means of low intensity UV LED irradiation is discussed.

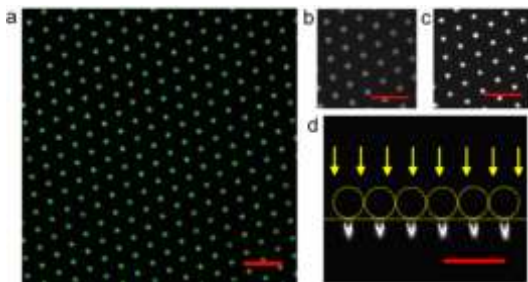


Fig. 1. Confocal microscope PL image of the periodic structure recorded by laser in photoinduced nanocomposite. [1]. Scale bar is 20 μm .

Aknowledgments. This work is supported by the Russian Foundation for Basic Research (Grant No. 19-02-00694 a).

[1] A. A. Smirnov, et. al., Opt. Mat. Express 10 (2020) 2114–2125.

HALL 1

T13-O: Quantum transport through a quantum dot side-coupled to a Majorana bound state pair in presence of electron-phonon interaction

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We theoretically investigate quantum transport through a quantum dot connected to Majorana bound states confined at the ends of a topological superconductor nanowire which forms a loop that is threaded by a magnetic flux.

The tunable magnetic flux allows one to manipulate the electron transport through the dot. We also study the phonon-assisted Majorana induced transport properties when the quantum dot is in interaction with a single long-wave optical phonon mode. The electron-phonon interaction is treated using a canonical transformation within the nonequilibrium Green's function formalism. The retarded Green's functions are calculated by applying the equation of motion technique. We find that when the two Majorana bound states are unhybridized, the zero-temperature linear conductance presents a 2π periodicity as a function of magnetic flux phase regardless the value of electron-phonon interaction, quantum

dot energy, or finite values of dot-Majorana couplings. When the Majorana bound states overlap, the linear conductance periodicity transforms to 4π either due to a finite electron-phonon coupling strength, or a tuned dot level. The differential conductance periodicity changes from 2π to 4π when the Majorana bound states hybridize and the electron-phonon coupling is finite. Our results show that the energy exchange with a single phonon mode, alters the Majorana-induced current signatures [1].

[1] L. Máthé, D. Sticlet, L. P. Zârbo, (2021) arXiv: 2107.05410.

T13-I: Scaling behavior of the momentum distribution of a quantum Coulomb system in a confining potential

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We calculate the single-particle momentum distribution of a quantum many-particle system in the presence of the Coulomb interaction and a confining potential.

The region of intermediate momenta, where the confining potential dominates, marks a crossover from a Gaussian distribution valid at low momenta to a power-law behavior valid at high momenta. We show that for all momenta the momentum distribution can be parametrized by a q-Gaussian distribution whose parameters are specified by the confining potential.

The real-space pair-correlation function calculated in this way can, in principle, be used to construct improved exchange-correlation functionals to solve electronic structure problems.

Furthermore, we find that the functional form of the probability of transitions between the confined ground state and the n^{th} excited state is invariant under scaling of the ratio Q_2/v_n , where Q is the transferred momentum and v_n is the corresponding excitation energy.

Using the scaling variable Q_2/v_n the maxima of the transition probabilities can also be expressed in terms of a q-Gaussian.

T13-I: Inverse Faraday effect in Mott insulators

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The inverse Faraday effect (IFE), where a static magnetization is induced by circularly polarized light, offers a promising route to ultrafast control of spin states. Here we study the inverse Faraday effect in Mott insulators using the Floquet theory. In the Mott insulators with inversion symmetry, we find that the effective magnetic field induced by the IFE couples ferromagnetically to the neighboring spins. While for the Mott insulators without inversion symmetry, the effective magnetic field due to IFE couples antiferromagnetically to the neighboring spins. We apply the theory to the spin-orbit coupled single- and multi-orbital Hubbard model that is relevant for the Kitaev quantum spin liquid materials and

demonstrate that the magnetic interactions can be tuned by light.

T13-PL: Neither a Metal, nor an Insulator: Stout Domain Walls Around the Mott Point

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Many Mott systems feature a first-order metal-insulator transition at finite temperatures, with an associated phase coexistence region displaying inhomogeneities and local phase separation. Here one typically finds "bubbles" or domains of the respective phases, which are separated by surprisingly thick, or stout, domain walls, as revealed both by imaging experiments and recent theoretical modeling. To gain insight into this unexpected behavior, we perform a systematic model study of the structure of such metal-insulator domain walls around the Mott point, within the Dynamical Mean-Field Theory framework. Our study reveals that a mechanism producing such "stout" domain walls can be traced to strong magnetic frustration, which is expected to be a robust feature of "spin-liquid" Mott systems.

T13-I: Electronic correlations and Fermi-liquid behavior of intermediate-band states in titanium-doped silicon

323

Andreas Oestlin¹

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We study the nature of the electronic states in the intermediate band formed by interstitial titanium in silicon. Our single-site description combines effects of electronic correlations, captured by dynamical mean-field theory, and disorder, modeled using the coherent potential approximation and the typical medium mean-field theory. For all studied concentrations an extended metallic state with a strongly depleted density of states at the Fermi level is obtained. The self-energy is characteristic to Fermi-liquids and for certain temperatures reveals the existence of coherent quasi-particles.

- 08:00 **Plenary Session**
HALL 1
- 10:20 Coffee Break
- 11:00 **Plenary and Invited Session**
HALL 1
- 12:35 Closing ceremony
- 13:20 Lunch
- 15:00 Excursion to Daly Museum

HALL 1

T9-PL: Interactions in the pre-AD mimicking model membranes

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Alzheimer's disease (AD) is a conformational disease caused by the formation of senile plaques, consisting primarily of amyloid-beta peptides. The crucial role in this process at its pre-clinical stage is likely imparted by peptide-membrane interactions. The experimental data suggest several intriguing structural properties of biomimetic membranes that modulate such interactions. First, it is their sensitivity to the charge present in the surrounding environment. The structure of membranes changes for example with increasing concentration of ions, which appears to be an effect born by peculiar properties of ions and lipid themselves. Interestingly, the differences in lipid interactions with ions have been linked to the hydration properties of the ions. A plausible mechanism of action in the case of many membrane additives seems to be in shifting the water encroachment the way that bilayers

absorb more or less water molecules. The hydration interactions appear to determine also the location of membrane constituents, such as cholesterol, melatonin, and amyloid-beta peptides. Moreover, cholesterol increases the order of lipid hydrocarbon chains while increasing the stiffness of the membrane, contrary to the fluidizing effect of melatonin. The observations based on the neutron scattering experiments and MD simulations keep proving to be important for studies on amyloid toxicity and the molecular mechanism of AD. For example, we have recently observed the changes in the membrane structural properties that were driven by the incorporation of the amyloid-beta peptide into the system. During the temperature changes, the system experienced transitions between the vesicular and bicelle-like objects. The membrane shape changes were also accompanied by dramatic changes in the membrane thickness. The conclusions of various investigations can thus provide an understanding for the possible structural changes taking place within biological membranes at the onset of AD.

Acknowledgement. This work has been supported by the Russian Science Foundation under grant 19-72-20186.

T6-PL: Silicon electronics at atomic and molecular scales

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Silicon electronics has been progressing at a fast, but steady pace over many decades by the continuous miniaturization of the electronic devices, such as transistors and diodes, along the

Moore's law. The foreseeable limits of Moore's law and the quest for new physics to incorporate in future devices for enhanced functionality have attracted interest in alternatives beyond miniaturization. We have pursued such a new research direction into atomic- and molecular-scale electronics by utilizing dopant atoms (or "molecules") in silicon, contributing to a field coined as dopant-based electronics. [1] This is based on the well-established platform of silicon nano-devices, but changing the active unit in transport (mainly by quantum tunneling) to dopant-atoms substitutionally embedded in the Si crystalline matrix. Along this approach, we fabricate, characterize and simulate ultimately-small Si devices (with dimensions on the order of ~ 10 nm), analyzing signatures of dopant-atoms. We will report single-electron tunneling (SET) in silicon-on-insulator nanodevices via individual donors [1,2] or via clusters of donors [3] working as quantum dots, not only in transistors, but also in tunnel diodes [4]. Focus will fall on illustrating how silicon nanoelectronics can naturally move forward in the fundamental dimensionalities at molecular and atomic scales, providing new perspectives for future generations of electronics, based on the Si platform, but with disruptive conceptual approaches. Acknowledgements: This work was partially supported by Grant-in-Aid for Scientific Research (JP19K04529) from MEXT, Japan, and a Cooperative Research Project of the Research Institute of Electronics, Shizuoka University.

[1] D. Moraru et al, Nano. Res. Lett. 6, 479 (2011).

[2] M. Tabe et al, Phys. Rev. Lett. 105, 016803 (2010).

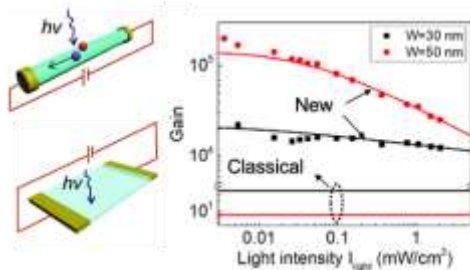
[3] D. Moraru et al, Nano. Res. Lett. 10, 377 (2015).

T1-PL: The device principle of low-dimensional high-gain phototransistors

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Low-dimensional photodetectors, in particular those in photoconductive mode, have been extensively investigated in past decades, including thin films[1], quantum dots[2], nanowires[3] and more recently two dimensional semiconductors.[4] The persistent research interests are mainly driven by the extraordinarily high photo gain (up to 10^{10} in quantum efficiency) observed in these devices. However, after decades of research, these devices are still poorly understood in terms of gain mechanism, transient and frequency responses. In this talk, I will present the research findings of my group in this filed in the past few years. I will first elaborate our finding that the classical device principle of photoconductors is derived on two misplaced assumptions.



Explicit Gain Equations for Low Dimensional Phototransistors

We then found a new device model for high-gain conductive photodetector based on photo Hall effect measurements. From

the device model, we established explicit gain equations for high-gain photoconductors that fit the experimental data well. In the end, we further derived the analytical transient photoresponses for high-gain photoconductors. These research findings offer us a better understanding of high-gain photoconductive devices and allow us to quantitatively design these in terms of photogain, bandwidth and dark current.

[1] N. Matsuo, et al, Jpn. J. Appl. Phys. 1984, 23, L299.

[2] V. Adinolfi, et al, Nature 2017, 542, 324.

[3] C. Soci, et al, J. Nanosci. and Nanotechnol. 2010, 10, 1430.

[4] J. H. Lee, et al, Nano Lett 2017, 17, 673

T10-PL: Harmonic generation in random nonlinear crystals: application to ultrashort pulse characterization and analysis of domain statistics

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¹*Department of Physics, Politechnic University of Catalonia, Barcelona, Spain*

We discuss the spatial distributed second harmonic (SH) generation from a disordered nonlinear crystal, having a random size and distribution of nonlinear domains with homogeneous refractive index. The distribution of the nonlinear domains generates a transverse SH signal emitted in all directions of the plane perpendicular to the propagation direction, with a similar efficiency over a very broad wavelength range, without the need of the phase matching condition. On the other hand, the crystal itself serves as a highly dispersive and ultra-broadband nonlinear medium, acting on the pulse propagating through it. We implement these nonlinear properties of such crystal in two applications. 1. Ultrashort pulse characterization. Precise characterization of ultrashort

laser pulses is a challenging task and a hot topic of research, since these lasers are nowadays implemented in advanced applications of different scientific and technological fields. We present a novel single shot auto-correlation technique, capable of measuring the most important parameters of an ultrashort laser pulse: pulse duration, chirp parameter, wave front tilt and the spectral phase. This method does not require phase matching condition nor sensitive alignment of thin nonlinear crystals and the same set-up can be used for the measurements of pulses with duration between 30 fs and 1 ps and wavelength in the range of 800 and 2000 nm.

2. Nondestructive analysis of disordered nonlinear domain statistic. The analysis of the SH spatial distribution can be implemented to an indirect, non-destructive optical method for domain statistic characterization in random nonlinear crystals. We apply this technique, based on a combination of numerical simulations and experimental measurements, to the characterization of different random media, with drastically different statistical distributions of ferroelectric domains. We have implemented and tested this method in crystals with different types of domain distributions. The analysis of the angular dependence of the SHG on the fundamental beam wavelength informs us about complicated domain structures. This method can be used for real time monitoring of the unknown domain distribution during crystal growth.

Online

T13-PL: Floquet-Bogoliubov approach for time-periodic driven Luttinger liquids

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Time-periodic driving facilitates a wealth of novel quantum states. The interplay of Floquet states and strong correlations is particularly intriguing. We therefore consider the exactly solvable Lieb-Liniger model of quasi-1D interacting bosonic atoms with time-periodically modulated interactions. By developing a time-periodic operator algebra for Luttinger liquids, we are able to obtain and analyze the complete set of explicit steady state solutions in terms of a Floquet-Bogoliubov ansatz and known analytic functions. When the driving frequency is lowered below the Luttinger liquid cutoff energy, a dramatic change of behavior is observed which is signaled by the appearance of strong resonant density waves. We discuss the situation in an experimental optical trap, but the theoretical results hold for general Luttinger liquids with time-periodic parameters.

T13-PL: From electronic structure theory to multiscale simulations of magnetisation dynamics

Olle Eriksson¹

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In this talk the complexities of theory of electronic structures of materials will be high-lighted, and the most common approximations for their calculations will be discussed. A multiscale step is then introduced, to show how one can perform simulations of magnetization dynamics, using hundreds of thousands of atoms, based on computational parameters obtained from electronic structure theory, using only one atom per cell. Examples from collective excitations, like magnons will be given, and it will be shown that quantum entanglement can be significant in these excitations. Finally, a final step in the multiscale simulations will be discussed, where a transition from the atomistic regime to a continuum model of the magnetization dynamics will be described, with examples from skyrmion dynamics and the influence of atomic defects.

T13-I: THz absorption at the interface between superconducting microwave devices and hydrogen crystals

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Microwave superconducting resonators made of patterned thin films are widely used for detectors and quantum computing. Aluminum is one of the most used materials,

thanks to its ease of fabrication and the fact that its surface, covered by a self-limiting native oxide, is stable in atmospheric conditions. One of the main sources of dissipation and frequency shifts in these devices is constituted by broken Cooper pairs, a significant part of which originate in interactions with THz radiation; be that stray or guided. I will present recent experiments which suggest that a very thin Hydrogen crystal deposited on the surface of the device can significantly shield against THz photons. The shielding effect is puzzling at first glance due to the fact that Hydrogen crystals are not active in this frequency range. Using molecular dynamics models we explain the results as absorption at the interface between the hydrogen crystal and the native aluminum oxide. Future devices could use this strategy to engineer efficient absorbing coatings for quantum devices or cryogenic band pass filters for kinetic inductance detectors.

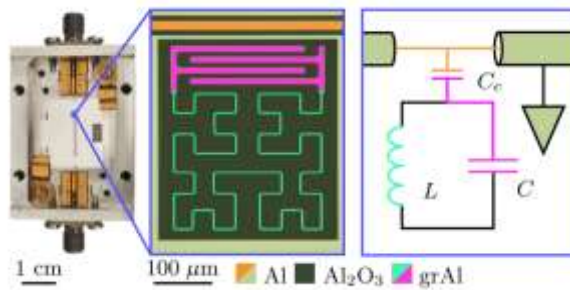


Fig. 1: Mounted chip (left) supporting 22 kinetic inductance detectors (center), modeled as lumped element circuits (right) [1]

[1] F. Valenti et al. Phys. Rev. App. 11 (2019) 054087.



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