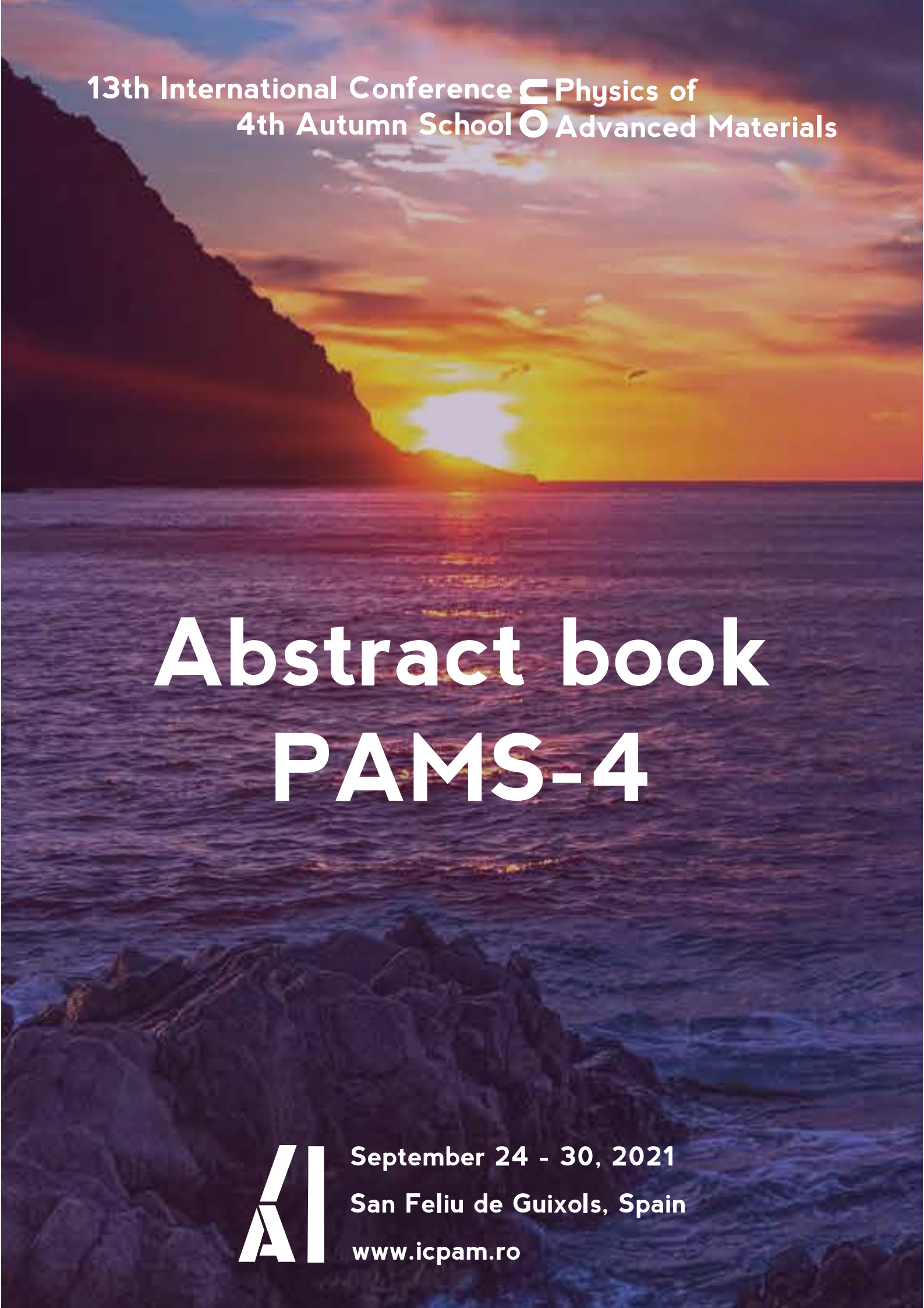
13th International Conference on Physics of
4th Autumn School on Advanced Materials
Abstract book
PAMS-4
September 24 - 30, 2021
San Feliu de Guixols, Spain
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PAMS-4

4th Autumn School on Physics of Advanced Materials

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

Daily Program and Abstracts

Cristina Pachiu

Mihaela Toma

Luminita Popa

Maria Ignat

Dragos Dutu

Cover: 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 Surfce 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 beggan 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 publishe 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, Helenic 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 Mediteraneo -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

J. de Rojas[1], E. Menéndez[1], J. Sort[1,2]

[1]*Physics Department, Universitat Autonoma de Barcelona, Bellaterra, Spain*
[2]*Institució Catalana de Recerca I Estudis Avançats (ICREA), Barcelona, Spain*

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 In_2O_3–based transparent conductive films

T. Yamamoto[1]

[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 ºC 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 In_2O_3-based films.[1-4] Recently, we reported Ce- and H-codoped In_2O_3 films (ICO:H) with a thickness of 100 nm showing high Hall mobility of 145 $cm^2/(Vs)$ with solid-phase crystallization: The films were deposited at a substrate temperature of 150 ºC by reactive plasma deposition with direct current arc discharge, subsequently were postanneled at 200 ºC 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-baesd 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 Teodorescu[1]

[1]*Surfaces 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 $Ug(\varepsilon F)>1$, where $g(\varepsilon)$ is the paramagnetic density of states (DOS), and εF 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: $(dg/d\varepsilon)(\varepsilon_F)\int_0^{\varepsilon_F} g(\varepsilon)d\varepsilon<g^2(\varepsilon_F)$. 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 whithout Cd, used in photovoltaics for terestrial and space applications

Stefan Antohe[1]

[1]Department of Electricity, Solid State and Biophysics, Faculty of Physics, University of Bucharest, 077125, Magurele-Ilfov, 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 hunders 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 illuminatioan 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 1014 protons/cm^2 and 1013 alpha particles/cm^2, 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 comparated. 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, Porceedings of the Romanian Academy, Series A, 22 (2021) 25–34.

T3-PL: Materials for low temperature fuel cells

Christophe Coutanceau[1]

[1]*Laboratory of Catalysis in Organic Chemistry (LACCO), University of Poitiers, France*

Hydrogen produced by water electrolysis from renewable energy sources (wind, solar, tidal, etc.) is expected to become a key energy vector to compete with fossil fuels. Due to his high energetic density (32.9 kWh/kg), one of the main targeted uses of clean hydrogen is the production of electricity through feeding of fuel cells, and particularly proton-exchange membrane fuel cells (PEMFCs) for transportation (cars, trucks, buses, trains, etc.) and cogeneration of heat and power (CHP for buildings, industries, isolated remote locations) application. But the spreading of PEMFC technology faces important issues, amongst them durability and cost represent strong limitations to commercialization.

Fuel cell stacks are composed of several unit cells connected in parallel or in series depending on the targeted stack outputs (voltage and current). These unit cells contain two electrodes, where electrochemical reactions occur on dedicated catalysts, the hydrogen oxidation reaction (HOR) at the anode and the oxygen reduction reaction (ORR) at the cathode, a proton conductive solid polymer as electrolyte and two bipolar plates as current collectors. The efficiency, feasibility, cost effectiveness, and durability of PEMFCs will greatly depend on the characteristics of these core materials used for their manufactures. The R&D effort on materials for PEMFCs has two main objectives: in short term to improve the performances (mainly efficiency and durability) of existing materials by proposing mitigation methods and in mid and long terms to

develop the next generation of materials and components for more durable and less costly systems, based on less strategic metals and more environmentally friendly compounds and processes.
In this contribution, the working principle of a PEMFC will be presented to point out the different phenomena and constraints that could alter the materials constituting the different components of the fuel cell core, and further the performance of the fuel cell in terms of efficiency and durability. Then the state-of-the-art materials will be presented, as well as the main directions for the development of future materials for the next generation of PEMFCs: catalysts and supports, proton-conductive polymers as solid electrolyte membranes between both electrodes and as ionomer impregnating the electrodes, and materials for the gas diffusion layers (GDLs).

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

A. Dinescu[1], M. Dragoman[1], D. Dragoman[2]

[1]*IMT Bucharest, Voluntari, Romania*
[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.

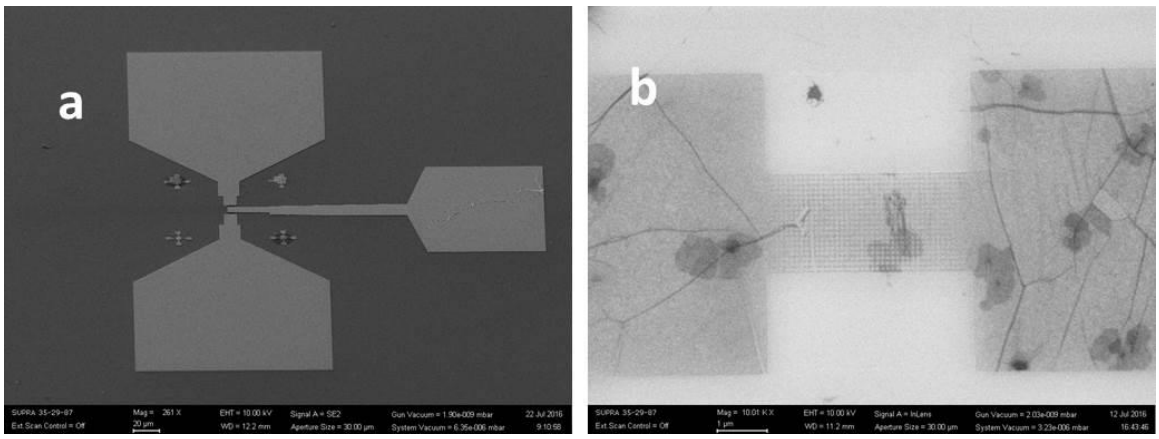


Fig. 1. Graphene based field effect transistor (a) and nanopatterned graphene channel (b)

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. Gavrila, A. Avram, R. Muller "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 Orfescu[1]

[1]*NanoArt21, 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.

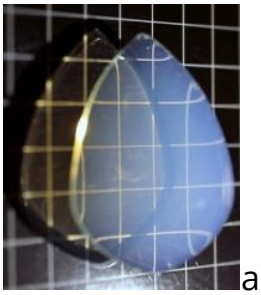
T12-I: The Sound of Nano: The nanomaterial silica aerogel as a priceless piece of sky for high jewellery design

Ioannis Michlaoudis[1]

[1] *American University of Cyprus (AUCY), Larnaka, Cyprus*

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.


a)

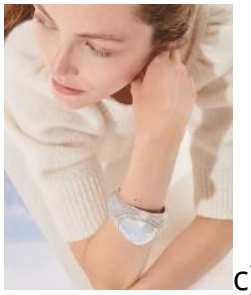
b)

c)

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 Davos[1],

[1]*Athens 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 Nanotecnology 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 “Weltanschaung”. 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 recurred to an artistic-like paradigm, or model of representation of his theories, to vulgarize, or explain plainly in a parroquial 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 Ursyn[1]

[1]*University of Northern Colorado, USA*

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. Lish[1]

[1]*American visual artist, DPhil candidate in Theoretical Physics at Oxford University*

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

Hermay NM, Santa Fe, NM, USA

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.

[1] T. Colding, W. Minicozzi, W. (2006*).* Proc. Nat. Acad. Sci. 103 (30) (2006) 11106-11111.
[2] A. Unwin, HDSR, https://doi.org/10.1162/99608f92.8ae4d525
[3] S. Bertschi et al. IEEE Xplore (2011) 329-336 http://doi.org/10.1109/IV.2011.58 .
[4] M. Agrawala, W. Li, F. Berthouzoz, Commun. ACM, 54 (4) (2011) 60-69 http://doi.org/10.1145/1924421.1924439

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

Christopher Sloan[1],

[1] *Maryland Institute College of Art in Baltimore*
[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

HALL 1

Poster Session PAMS-4

Online

PAMS-P Modification of the plasmonic properties of AuNPs photoactivated and stabilized in lipid-chitosan; preliminary data

E. Olteanu[1], D. Pricop[1], A. Les[1]

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

The AuNP study has proved extremely promising in medical research and has led to the search for the best solutions in their optimization [1]. Their effectiveness may depend on the degree of biocompatibility, cell turnover and especially the level of internalization in the target cells. One of the methods of optimizing AuNP is related to the control of size and surface chemistry. In this paper we studied the plasmonic activity of AuNP photoactivated and functionalized with lipid and

chitosan. AuNP photoactivated in visible light and coated with a layer of lipid showed an increase in LSPR intensity, and a moderate stability of the suspension. By coating with chitosan the level of stability increased but there was a decrease in LSPR. Following dialysis, the suspensions generally tended to agglomerate, with the exception of lipid and chitosan-coated AuNP suspensions which proved to remain particularly stable after more than 2 months, even at room temperature. The analyzes suggested a stronger binding of chitosan to the surface of photoactivated nanoparticles in visible light, compared to those that were not photoactivated. Acknowledgement. Part of this research was supported by J.I.N.R. Dubna projects, 2021

[1] A. Bhat, L. W. Edwards, X. Fu, D L. Badman, S. Huo, A. J. Jin, Q. Lu Appl Phys Lett. 109 (26) (2016) 263106.

PAMS-P Physical properties of ultra thin photovoltaic structures based on AII-BVI compounds

A.-M. Panaitescu[1], V.-A. Antohe[1,2], S. Iftimie[1], A.-M. Raduta[1], A. Radu[1], L. Ion[1], S. Antohe[1,3]

[1]Department of Electricity, Solid-State Physics and Biophysics, University of Bucharest, Faculty of Physics, Bucharest-Magurele, Romania
[2]Institute of Condensed Matter and Nanosciences, Université catholique de Louvain (UCLouvain), Louvain-la-Neuve, Belgium
[3]Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest, Romania

A submicrometric multilayered structure for photovoltaic applications were prepared and characterized. Onto the optical glass an 100 nm silver (Ag) thin film, followed by 60 nm zinc phthalocyanine (ZnPc), were both deposited by vacuum

thermal evaporation (VTE) to obtain the hole colector electrode of the structures. On these electrodes 100 nm zinc telluride (ZnTe), 500 nm cadmium telluride (CdTe), were deposited to form the main absorber of the structures, and further a very thin film of cadmium sulfide (CdS) was deposited for the windows layer of the structure. The top electrode serving as TCO, was formed by very thin zinc oxide (ZnO) and indium tin oxide (ITO) thin films leading finally to the (Ag/ZnPc/ZnTe/CdTe/CdS/ZnO/ITO) submicrometric structures. All the ultra thin films were deposited by magnetron sputtering (MS) technique, apart from Ag and ZnPc layers. Subsequent structural chracterization through X-Ray diffraction (XRD) along with morphological investigation via atomic force microscopy (AFM) and scanning electron microscopy (SEM), and optical characterization by UV-VIS spectroscopy were performed on all structure's ultra thin films. The electrical measurements onto Ag/ZnPc/ZnTe/CdTe/CdS/ZnO/ITO revealed an asymmetrical dark current-voltage characteristics and good photovoltaic response at AM 1.5 illumination. The typical parameters of the structures obtained in regime of photoelement are: 400 mV for open circuit voltage (VOC), 73.6μA/cm2 for short-circuit current density (JSC) and 19.68% for the fill-factor.

PAMS-P: Flexible electrospun polyvinylidene fluoride separators for supercapacitors

D. Patlun[1], V. Khomenko[1], C. Gualandi[2] and M. Zanoni[2]

[1]Department for Electrochemical Power Engineering and Chemistry, Kyiv National University of Technologies and Design/ Kyiv, Ukraine

[2]Department of Chemistry "Giacomo Ciamician", University of Bologna, Via Selmi, 2, 40126 Bologna, Italy

Supercapacitors are used to store an electrical charge with a high power density and having a long life cycle compared to other storage devices. There is a strong interest to replace aqueous and organic electrolytes with ionic liquids (ILs) in supercapacitors to achieve high operating voltages and hence high energy density. ILs can overcome many disadvantages of conventional electrolytes, such as narrow potential windows, volatility, and especially flammability. However, ILs are very viscous relative to organic solvents and aqueous media. The higher ionic resistance is associated with poor electrolyte absorption by separators due to their viscosity. The ionic conductivity is a significant parameter for the electrochemical performance of supercapacitors. Here, we chose flexible electrospun polyvinylidene fluoride (PVDF) separators to evaluate their effect on performance and cell energy density. The electrospun mats were produced using a home-made electrospinning apparatus composed by a SL 50 P10/CE/230 high voltage power supplier (Spellman, New York, USA), a KDS-200 syringe pump (KD Scientific Inc., Massachusetts, USA), a glass syringe containing the polymer solution, a stainless-steel blunt-ended needle (inner diameter 0.51 mm, Hamilton, Bonaduz, Switzerland) connected with the power supply electrode and a grounded aluminum collector. The polymer solution was ejected at a flow rate of 1.2 $mL \cdot h^{-1}$, the needle was placed 23 cm away from the collector and the applied voltage was set at 17 kV. PVDF separator were prepared from a 18% (w/v) solution of PVDF dissolved in Ac:DMF=60:40 (v/v). Electrospinning was performed at room temperature and relative humidity in the range 40-50%. Membrane thickness

was about 70 μm. Morphological characterizations of the PVdF nanofiber separators by scanning electron microscopy (SEM) show that the nanoscale fiber structures have a diameter range of 720 ± 180 nm. The distribution of fiber diameters was determined through the measurement of about 300 fibers. The highly porous structure of electrospun PVDF separators (Fig.1) leads to better electrolyte uptake and wettability, lower resistance, and higher rate performance than Celgard one.

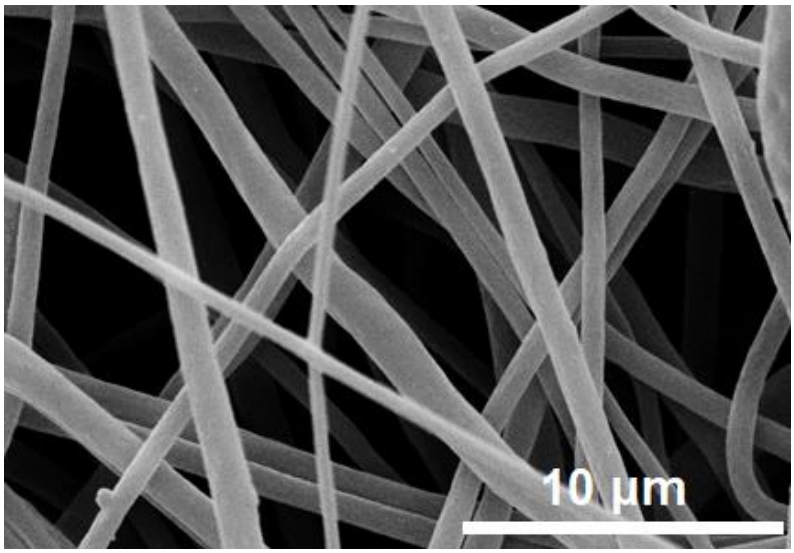


Fig. 1. High-magnification image of PVDF nano-fiber-based nonwoven material prepared by electrospinning, imaged with a SEM (Leica Cambridge Stereoscan 360) at an accelerating voltage of 20 kV

Electrospun PVDF and monolayer polypropylene Celgard 2400 separators were soaked in N-alkyl-N-butylpyrrolidinium bis(trifluoromethylsulfonyl)imide (Pyr14TFSI) ionic liquid before assembled in supercapacitors. The Nyquist plot for the two separators with ionic resistance of approximately 4.5 Ω and 48.6 Ω for electrospun PVDF and Celgard 2400, respectively. The higher resistance in Celgard 2400 is due to poor wettability by IL. Thus, electrospun PVDF separator demonstrated better

electrolyte wettability and ~10 times less resistance. As a result, it enabled superior rate performance of supercapacitors based on ILs.

Acknowledgements. The authors acknowledge the NATO Science for Peace and Security Programme, which supports this work under grant SPS G5772.

PAMS-P: 3D printed metal oxide-polymer composite materials for antifouling applications

A. Bouranta[1], N. Vrithias[2], G. Kenanakis[2], E. Sfakaki[3], N. Mitrizakis[3], C. Strakantounas[3], N. Papandroulakis[3], C. Romanitan[4], C. Pachiu[4], L. Barbu[5,6], M. P. Suchea[1,4], E. Koudoumas[1]

[1]Center of Materials Technology and Photonics, Hellenic Mediterranean University, Heraklion, 71410, Greece
[2]Institute of Electronic Structure and Laser, Foundation for Research & Technology-Hellas, N. Plastira 100, 70013, Heraklion, Greece
[3]Institute of Marine Biology, Biotechnology and Aquaculture, Hellenic Centre for Marine Research, Thalassocosmos, P.C. 71500, Gournes Heraklion, Greece
[4]National Institute for Research and Development in Microtechnologies , IMT-Bucharest, 1 26 A, Erou Iancu Nicolae Street, P.O. Box 38-160, 023573 Bucharest , Romania
[5]Electron Microscopy Center "Prof. C. Craciun", Faculty of Biology & Geology, "Babes-Bolyai" University, Cluj-Napoca, 400006, Romania
[6]Electron Microscopy Integrated Laboratory, National Institute for R&D of Isotopic and Molecular Technologies, Cluj-Napoca, 400293, Romania

Current technology to prevent biofouling relies on the use of toxic, biocide-containing materials, which can become a serious threat to marine ecosystems, affecting both targeted and nontargeted organisms [1]. The development of broad-spectrum, nontoxic antifouling materials is a challenge for researchers, since these can be quite important in applications

like aquaculture [2,3]. In that respect, surface chemistry, physical properties, durability and attachment scheme can play a vital role in the performance of the materials. Acrylonitrile butadiene styrene (ABS) / metal oxides (MO) composite lattices of different MO content were developed using 3D printing and their applicability in aquaculture was examined. All fabricated materials were studied using X-ray diffraction, electron microscopy and Raman spectroscopy, while their antifouling action was investigated by monitoring the growth of the diatoms Navicula sp. and the monocellular algae *Chlorella sp* on them. For this investigation, a chamber was employed, where the plankton cultures were maintained in constant conditions (temperature, light, aeration) the samples being placed within the cultures for a period of 15 days, when the area covered with algae was estimated applying image analysis techniques.

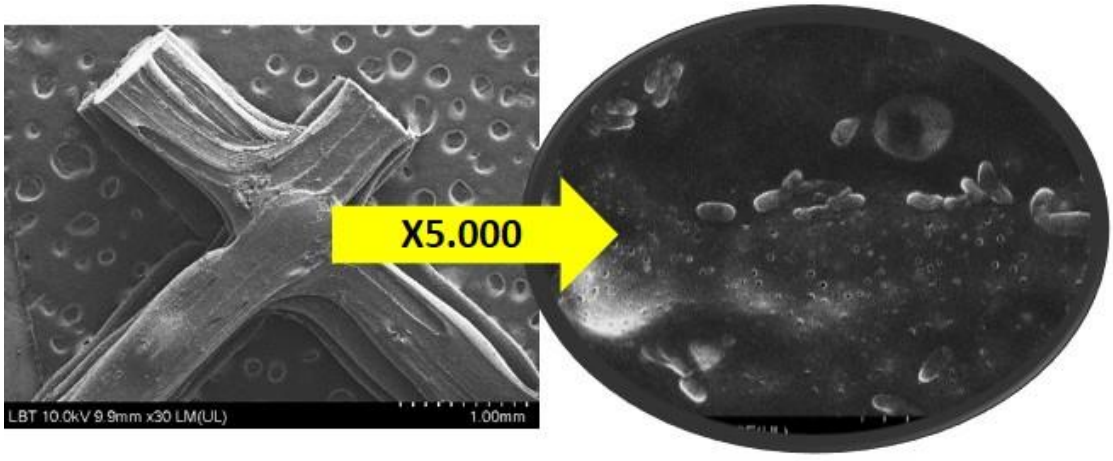


Fig.1. The image shows a SEM image of a ZnO/ABS 3D printed grid coated with biofilm and a detail of it.

Studies showed promising results but further material improvements are needed. In particular, the MO concentration

in the composite materials was found to control the antifouling ability (Fig.1).

[1] N. Bloecher et al., Aquaculture, 519 (2020) 734936.
[2] J. Bannister et al, , Biofouling, 35(6) (2019) 631–648.
[3] F. Oppedal et al, , Aquaculture, 315(3) (2011) 361–368.

PAMS-P: Comparative study of electrochromic V_2O_5 and WO_3 films grown by spray pyrolysis

K. Mouratis[1,4], I. V. Tudose[1,5,6], C. Romanitan[2], M. Popescu[2], G. Simistiras[1,3], S. Couris[4], M. P. Suchea[1,2] and E. Koudoumas[1,3]

[1] *Center of Materials Technology and Photonics, School of Engineering, Hellenic Mediterranean University, 71410 Heraklion, Crete, Greece*
[2] *National Institute for Research and Development in Microtechnologies - IMT Bucharest, 126A, Erou Iancu Nicolae Street, 077190, Voluntari-Bucharest, Romania*
[3] *Department of Electrical and Computer Engineering, School of Engineering, Hellenic Mediterranean University, 71410 Heraklion, Crete, Greece*
[4] *Physics Department, University of Patras, 26500 Patras, Greece*
[5] *Chemistry Department, University of Crete, Heraklion, Greece*
[6] *IESL-FORTH, Heraklion, Crete, Greece*

Among other materials, tungsten trioxide (WO_3) and vanadium pentroxide (V_2O_5) are the most promising materials for electrochromic applications and they both have been widely studied [1–3]. The present contribution concerns a comparative study of electrochromic WO_3 and V_2O_5 films with novel (mixed wall-like/granular) surface structuring, fabricated by the spray pyrolysis technique onto FTO substrates. Films of similar thikness, grown under similar conditions were developed and fully characterized, with respect to their structural, morphological and electrochromic properties, employing XRD, SEM, Raman spectroscopy, UV-Vis spectroscopy and cyclic

voltammetry- chronoamperommetry. The investigation was focused on the correlation between the surface morphology of the samples and their electrochromic performance.

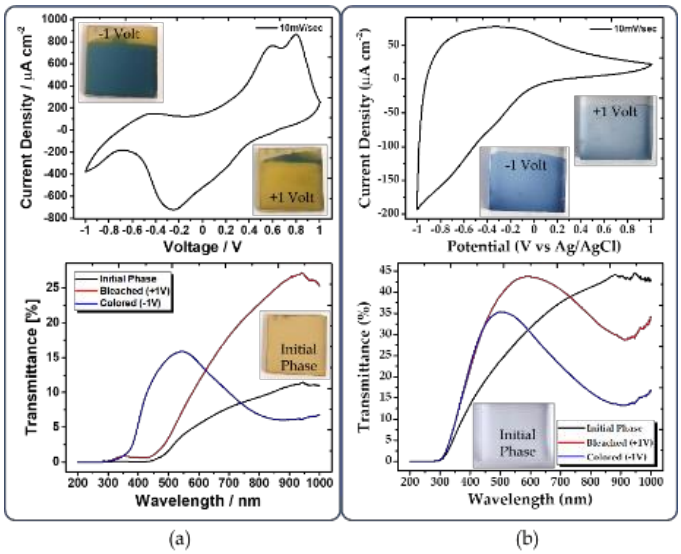


Fig. 1. The image shows the color change, uv-vis spectrum and cyclic voltammetry mesurements for a V_2O_5 (a) and a WO_3 (b) film.

The following images show an example of the samples studied and their electrochromic performance, the targeting being the comparison between V_2O_5 and WO_3 films. Further studies for improving and optimizing the electrochromic performances are ongoing.

[1] K. Mouratis et al, Mater 13(17) (2020) 3859.
[2] K. Mouratis et al, Nanomater 10(12) (2020) 2937.
[3] C. Pachiu et al, Proc. Int. Semicond. Conf. CAS (2020) 191-194.

Sunday, September 26, 2021

08:00	**Plenary and Invited Session** HALL 1
10:20	Coffee Break
11:00	**Invited Lectures** HALL 2 – Salon Goya
13:35	Lunch
15:00	**Invited Lectures** HALL 2
17:55	Coffee Break
18:30	**Invited and Oral Session** HALL 1
20:30	Dinner

HALL 1

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

José María De Teresa[1]

[1]*Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain*

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].

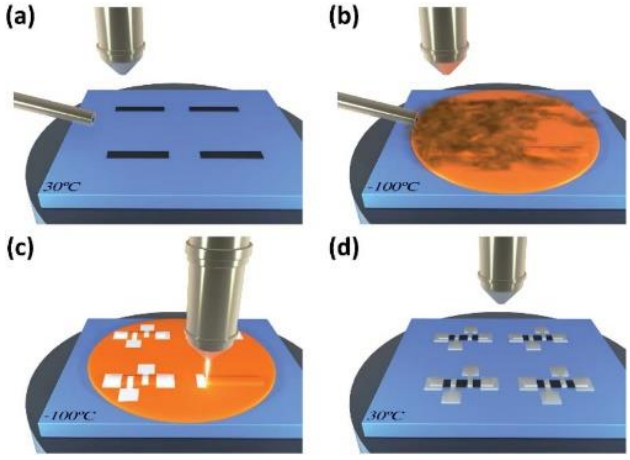


Fig.1. Cryo-FIBID process used to grow electrical contacts on 2D materials (e.g., graphene).

The third application is based on the use of FIBID under cryogenic conditions (Cryo-FIBID, Fig.1), 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).

[1] Nanofabrication: nanolithography techniques and their applications, J. M. De Teresa, Institute of Physics, UK, 2020.
[2] M. Jaafar et al., Nanoscale 12, 10090 (2020)
[3] P. Orús et al., Nanotechnology 32, 085301 (2021)

T14-PL: Chalcogenide materials development for infrared sensor innovations

V. Nazabal[1,3], J. Charrier[2], M. Baillieul[1,3,4], J. Ari[1], F. Starecki[1,5], C. Boussard-Pledel[1], L. Bodiou[2], A. Braud[5], P. Němec[3], E. Rinner[4], K. Michel[6]

[1]ISCR, University of Rennes 1, France
[2] FOTON, University of Rennes 1, France
[3]University of Pardubice, Czech Republic
[4]IFREMER, Plouzané, France
[5]CIMAP, University of Caen, France
[6]BRGM, Orléans, France

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 CGSµLAB, 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

G.F. Goya[1,2,3], C. Marquina[1,2,3], M. R. Ibarra[1,2,3]

[1]Institute of Nanoscience and Material of Aragon (INMA), University of Zaragoza and CSIC, Spain

[1]Laboratory of Advanced Microscopies, University of Zaragoza, Spain

[1]Department 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 led 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].

[1] M. Arruebo, R. Fernandez-Pacheco, M.R. Ibarra, J. Santamaria Nano Today 2(3) (2007) 22-32

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[3] L. Asín, M. R. Ibarra, A. Tres and G. F. Goya. Pharm. Res. 29(5), 2012, 1319-1327.

[4] by M. P. Calatayud, L. Asin, A. Tres, G.F. Goya, M.R. Ibarra. Current Nanosci. 2016, 12(3) 372-37

[5] M.P. Calatayud, E. Soler, T.E. Torres, E. Campos-Gonzalez, C. Junquera, M.R. Ibarra, G.F. Goya. Sci. Rep. 7 (1) 8627 (2017).
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[7] B. Sanz, M.P. Calatayud, T.E. Torres, M.L. Fanarraga, M.R. Ibarra and G.F. Goya. Biomaterials 114 (Jan 2017) 62–70.
[8] C. Marquina, M.R. Ibarra, in: P.K. Zarzycki (Ed.), Pure and Functionalized Carbon Based Nanomaterials, CRC Press2020.
[9] R. Fernandez-Pacheco et al, J. Magn. Magn. Mater. 311(1) (2007) 318-322.

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

Dimitris Tsoukalas[1]

[1]*Dept. of Applied Physics, National Technical University of Athens, Athens, Greece*

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].

[1] P. Bousoulas, D. Sakellaropoulos, D. Tsoukalas, Applied Physics Letters 118 (14), 143502 (2021)
[2] D. Sakellaropoulos et al., IEEE Electron Device Letters 41, 7, (2020)

Invited Lectures

HALL 2

PAMS-IL: The device principle of high gain photoconductors

Yaping Dan[1]

[1] *University of Michigan - Shanghai Jiao Tong University Joint Institute, Shanghai Jiao Tong University, Shanghai, China*

Photoconductors as the simplest photodetectors have been extensively investigated on various semiconducting materials in the past 60 years including thin films, nanowires, quantum dots, and more recently twodimensional (2D) atomic layers (Fig.1). The persistent research interests in photoconductors for decades are mainly driven by the extraordinarily high gain in quantum efficiency (up to 10^{10}) observed in these photoconductors. However, the device principle of these photoconductors is still poorly understood after decades of research. 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. We then found a new device model for high-gain phtoconductors 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 phtoconductors and allow us to quantiatively design photoconductors in terms of photogain, bandwidth and dark current.

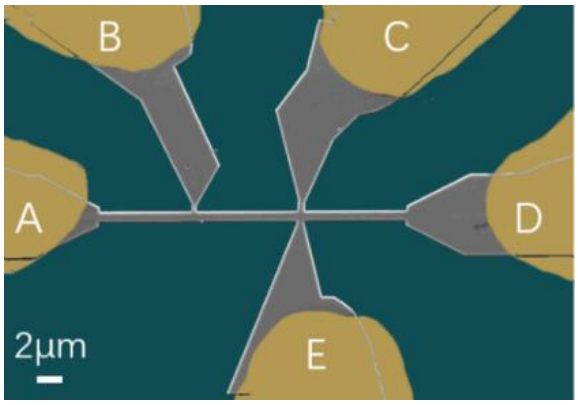

Fig.1. Nanowire photoconductors

PAMS-IL: A new generation of semiconductors: metal oxides

E. Fortunato[1], E. Carlos[1], R. Branquinho[1], P. Barquinha[1], R. Martins[1]

[1]Materials Science Department, CENIMAT|I3N and CEMOP/UNINOVA, Faculty of Sciences and Technology, NOVA University Lisbon, Portugal.

Oxide electronic materials is one of the most promising technologies for electronic devices, as distinct from the

traditional silicon technology. The fact that circuits based on conventional semiconductors such as silicon and conductors such as copper can be made transparent by using different materials, the so-called transparent semiconducting and conducting oxides (TSOs and TCOs, respectively), is of great importance and allows for the definition of innovative fields of application with high added value.

Oxide electronic materials are becoming increasingly important in a wide range of applications including transparent electronics, optoelectronics, magnetoelectronics, photonics, spintronics, thermoelectrics, piezoelectrics, power harvesting, hydrogen storage and environmental waste management. Synthesis and fabrication of these materials, as well as processing into particular device structures to suit a specific application is still a challenge. Further, characterization of these materials to understand the tunability of their properties and the novel properties that evolve due to their nanostructured nature is another facet of the challenge.

In this paper we will present the most important landmarks achieved by these stimulating scientific area as well as some insights to emerging applications.

PAMS-IL: ERC: A Way to Capture Talents

Rodrigo Martins[1,2]

[1]i3N/CENIMAT, Department of Materials Science, Faculty of Science and Technology, Universidade NOVA de Lisboa and CEMOP/UNINOVA, Campus de Caparica 2829-516 Caparica, Portugal

[2]Member of the Scientific Council of the European Research Council

As member of the scientific council of the European Research council, the aim of this presentation is to show the European Research Council mission to raise the level, dynamism, and creativity of the whole European research system by supporting the emergence of research leaders, improving the career prospects of early-stage researchers, and providing a benchmark for all of Europe's national research authorities and individual institutions, where science excellence is the only criterion. Along the presentation the way how talents are capture and their role in impacting in the challenges of the future, with practical examples of this excellency.

Invited Lectures

HALL 2

PAMS-IL: Proving nanoscale chiral interactions between cyclodextrins and propranolol enantiomers by means of SERS. Highlighting the key role played by the plasmonic substrate.

Rares Stiufiuc[1,2]

[1]*Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania*
[2]*Faculty of Pharmacy, University of Medicine and Pharmacy, Cluj-Napoca, Romania*

Chiral separation of pharmaceutical enantiomers is a very important issue especially for pharmaceutical industry. Over the year several methods have been developed for this purpose mainly based on chromatography. The working principle of this separation technique is based on the formation

of a transient diastereoisomer. However, the very subtle nanoscale interactions responsible for the separation are not always well understood. Over the last decade Raman and its counterpart (surface-enhanced) Raman spectroscopy have provided promising results for this topic but there are a lot of problems that still need to be solved. In this paper we present Raman/SERS experimental data that provide very useful information concerning the nanoscale interactions between the two enantiomers of Propranolol and the naturally occurring α, β, and γ cyclodextrins. Firstly, the Raman spectroscopy has been used to proof the successful formation of host-guest intermolecular complexes having different geometries of interaction. The occurrence of new vibrational bands specific to propranolol together with a change in the intensities of other bands are direct proofs of complexes formation. These experimental evidences have been also confirmed by quantum chemical calculations. Secondly, by performing SERS measurements on a new type of solid plasmonic substrate we were able to experimentally prove the intermolecular interactions responsible for chiral discrimination of PRNL enantiomers by cyclodextrins by means of SERS. It turned out that the interaction strength between the plasmonic substrate and the intermolecular complexes is of paramount importance for SERS based chiral discrimination. This approach could represent a very good starting point for the evaluation of molecular interactions manifesting between other pharmaceutical compounds and different classes of chiral selectands.

PAMS-IL: Non-destructive techniques to investigate the deffects in thin films

Stefan Antohe[1]

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

The space-charge-limited-currents (SCLC), appear when the density of free charge carriers injected from electrodes into volume of semiconducting material is higher than the thermal excited intrinsic charge carrier density of the semiconductor. The Current-Voltage (IV) characteristics of the SCL-currents change as a function of density and energetical distribution of defects into the semiconductor bandgap (BG). Knowing the analytical relationships of SCLC I-V characteristics for different trap distributions, the intrinsic and extrinsic charge carrier transport parameters could be determined by fitting the measured I-V characteristics with these analytical relationships. In this way we can talk about a nondestructive investigation technique of semiconducting materials based on simple measurements of I-V characteristics.
More quantitative information on the defects present into the semiconductor BG can be achieved from the thermo stimulated currents (TSC) spectra analysis and because of this a detailed description of the TSC will be presented too. As example of the application of these defect investigation techniques, the electrical properties of the non-irradiated and electron irradiated structures, containing polycrystalline thin layers of CdS and CdSe, are investigated. The thin films of CdS and CdSe were obtained through thermal-vacuum evaporation on the glass substrate at temperature of 220 °C. After the investigation of their structure by X-ray diffraction (XRD), the samples were subjected to two sessions of irradiation with 7 MeV electrons to different fluencies. The current-voltage characteristics,

recorded at temperatures in the range 150÷400 K, showed that the Ohm's law is followed at low-applied voltages, in both non-irradiated and irradiated CdS and CdSe layers. In the range of high-applied voltages, the space-charge-limited-current (SCLC), controlled by different types of trap distribution, placed in the bandgape of the semiconducting layer, has been identified as the dominant conduction mechanism. An analysis in the frame of SCLC theory allowed us to obtain the parameters characterizing the trap distributions and the changes induced by electron irradiation. For a better accuracy other technique like TSC, photoconduction spectra were used to characterize the irradiation induced defects. The defects determining the electrical properties of CdSe thin films, before and after irradiation with high-energy electrons, are presented. The main defect (D1), controlling the electrical properties of the films both before and after irradiation, is located at 0.38 eV below the conduction band edge. Some other defects, existing in lower densities and having lower ionization energies (0.24 eV - D2, 0.17 eV - D3 and 0.14 eV - D4) were also identified. Electron irradiation induces a significant increase of the peaks associated to the defects D1, D2 and D3, especially of the first one. The parameters characterizing all the detected traps are determined.

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[8] L. Ion, S. Iftimie, A. Radu, V. A. Antohe, O. Toma, S. Antohe, Proc. Rom. Acad. - Math. Phys. Tech. Sci. Inf. Sci. 22 (2021) 25–34.

PAMS-IL: Applications of dielectric colloidal microparticles in the field of laser-matter interaction

N. Bityurin[1], A. Pikulin[1], A. Afanasiev[1], V. Kamensky[1]

[1]*Instutuite of Applied Physics RAS, Nizhny Novgorod, Russia,*

We consider the problem of light diffraction on a dielectric sphere, photonic jets (Fig. 1) and spots formed in the near field of a microsphere, the features of nanostructures formed by laser irradiation of the set of dielectric microspheres placed on dielectric surfaces. We present the results on two-color irradiation of the layer of dielectric colloidal microparticles deposited on the dielectric surface by femtosecond pulses as well as opportunities offered by the irradiation of such layer by several coherent beams.

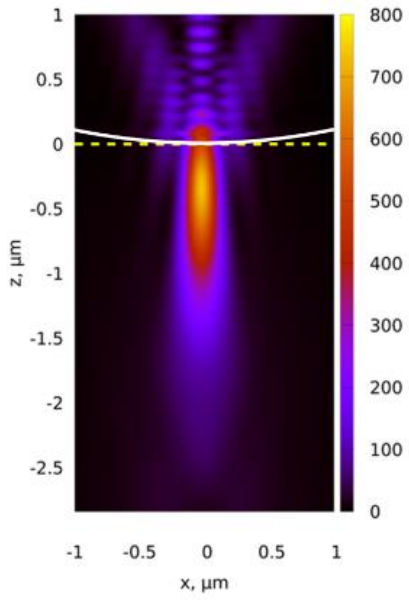

Fig. 1. FDTD calculation of the electric field square enhancement near the surface of one sphere within the close-packed array.

The employment of the layer of the colloidal microparticles as a light-acoustic convertor is discussed.

Aknowledgments.This work is supported by the Russian Foundation for Basic Research (Grant No. 19-02-00694 a).

PAMS-IL: Photoelectron spectroscopy: relevant information which can be extracted

Cristian Mihail Teodorescu[1],

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

This lecture will offer a practical introduction in photoelectron spectroscopies. After a first review of atomic physics, energy levels in atoms and in ionized species will be discussed, emphasizing the ability of this technique to provide elemental and chemical analysis of materials. The surface sensitivity is another aspect that will be discussed, together with relevant approaches for depth profiling of materials. The fourth aspect is related to the ability of this technique to analyze band bending occurring at interfaces and at free surfaces, in particular the ability to investigate free ferroelectric surfaces in a non-invasive way. The fifth feature of photoelectron spectroscopy is related to the ability of this technique to investigate samples with sub-micron lateral resolution, i. e. performing photoelectron spectro-microscopy. The sixth aspect will be related to photoelectron diffraction techniques, which provide with sub-Ångström accuracy geometries of adsorbates on surfaces or positions of impurities in the crystalline lattice. The seventh technique that will be discussed is valence band spectroscopy with angular resolution, a

technique able to reveal the dispersion laws of electrons in various materials. This technique may also be performed with spin resolution. Modern synchrotron radiation facilities offer very often all the above abilities, including the possibility for real time analysis of surfaces and thin films, with in situ observation of chemical reactions, or electronic or atomic structure changes, or changes in ferroelectric or ferromagnetism of the investigated samples. Several recent examples will be discussed [1].

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Invited and Oral Session

HALL 1

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

J. Lancok[1], S. Cichon[1], O. Heczko[1], E. de Prado[1], M. Veis[2], J. Hamrle[2]

[1]1Department of Analyses of Functional Materials , Institute of Physics CAS, Prague, Czech Republic
[2]Faculty of Mathematics and Physics, Charles University in Prague, Prague, Czech Republic

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 magnetooptical characterisations.

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

Georgeta Salvan[1]

[1]*Semiconductor Physics, Chemnitz University of Technology, Chemnitz, Germany*

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

S. Cichon[1], F. Maca[1], C. Drasar[2], J. Navratil[2], P. Cermak[2], V. Chab[1], J. Lancok[1]

[1]Department of Analysis of Functional Materials, Institute of Physics, the Czech Academy of Sciences, Prague, Czechia
[2]Faculty of Chemical Technology, University of Pardubice, Pardubice, Czechia

Topological insulator materials are gaining more and more interest due to their applications in spintronics [1-3]. In this study, bulk single crystal MxBi2-xSe3 (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.

Ebinding vs kǁ 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. Fe0.02Bi1.98Se3 displays band gap opening with the magnitude of around 0.1 eV.

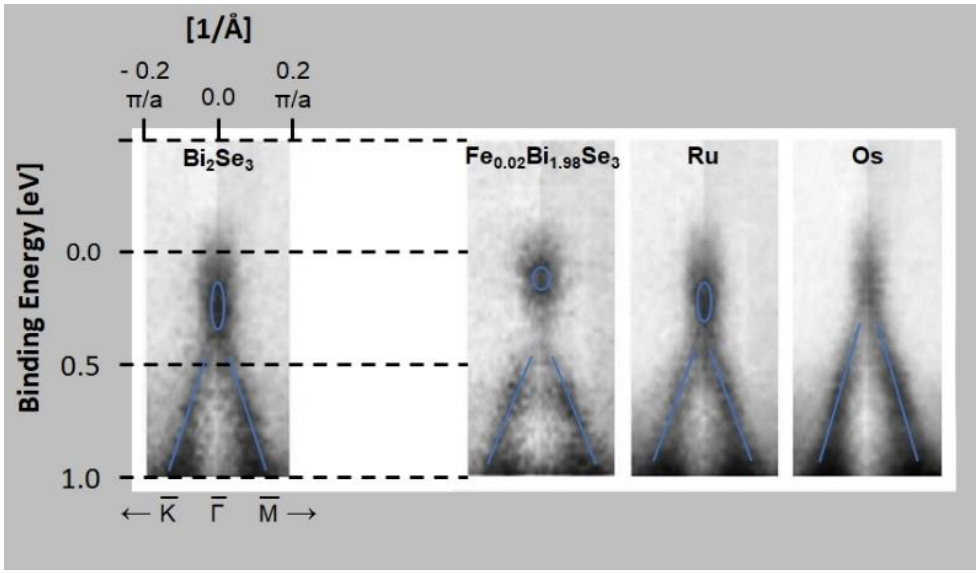

Figure 1. Measured Dirac cone structures. Dirac features and contribution form bulk conduction band are highlighted.

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 $CoFe_2O_4$ Nanoparticles

R. Bortnic[1], A. Szatmári[1], G. Souca[1], R. Dudric[1], R. Stiufiuc[2], A. Moldovan[2], I. Deac[1], E. Burzo[1], R. Tetean[1]

[1]*Faculty of Physics, Babes-Bolyai University, Cluj Napoca, Romania*
[2]*Department of Bionanoscopy, MedFuture Research Center for Advance Medicine,, "Iuliu Hatieganu" University of Medicine and Pharmacy, Cluj Napoca, Romania*

The magnetic $CoFe_2O_4$ 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 $Fd\bar{3}m$ space group with the lattice parameter a = 8.38 Å. 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 $M(t)/M(0) = A \exp(-E_a/k_BT)$. 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

R. Bosinceanu[1], A. Vasile[1], E. Vasile[1], I. Deac[3], M.N. Palamaru[1], A.R. Iordan[1], M. Iacob[4], 4 S. Ando[5], M. cazacu[6], D. Toloman, A. Popa, F. Iacomi[1]

[1]Faculty of Physics, Alexandru Iloan Cuza Uniiversity of iasi, Romania
Faculty of Chemistry, Alexandru Ioan Cuza of Iasi
[2]METAV S.A, Research and Development, Bucharest, Romania
[3]Faculty of Physics, Babes-Bolyai University of Iasi, Romania
[4]Institute of Chemistry of Moldavian Academy of Sciences, Republic of Moldova
[5]Tokyo University of Science, Japan
[6]Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania

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 and Mossbauer spectroscopies were used

to study the distribution, the content of iron oxides and the interaction between magnetic nanoparticles.

Monday, September 27, 2021

08:00	**Plenary Invited and Oral Session** HALL-1
10:20	Coffee Break
11:00	**Invited Lectures** HALL 2
13:35	Lunch
14:00	Excursion to Girona
20:00	Dinner

HALL 1

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

V. Nadtochenko[1,2], D. Cherepanov[1], A. Kostrov[1], F. Gostev[1], I. Shelaev[1], A. Gulin[1], A. Aybush[1], S. Kochev[3], Y. Kabachii[3]

[1]N.N. Semenov Federal Research Center for Chemical Physics, RAS, Kosygin St. 4, Moscow, Russian Federation 119991
[2]Department of Chemistry, Lomonosov Moscow State University, Leninskiye Gory 1-3, Moscow, Russian Federation, Russian Federation, 119991
[3]A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Vavilova St. 28, Moscow, Russian Federation, 119991

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 Mn^{2+}: $Zn_{\sim 0.5}Cd_{\sim 0.5}S/ZnS$ 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. 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.

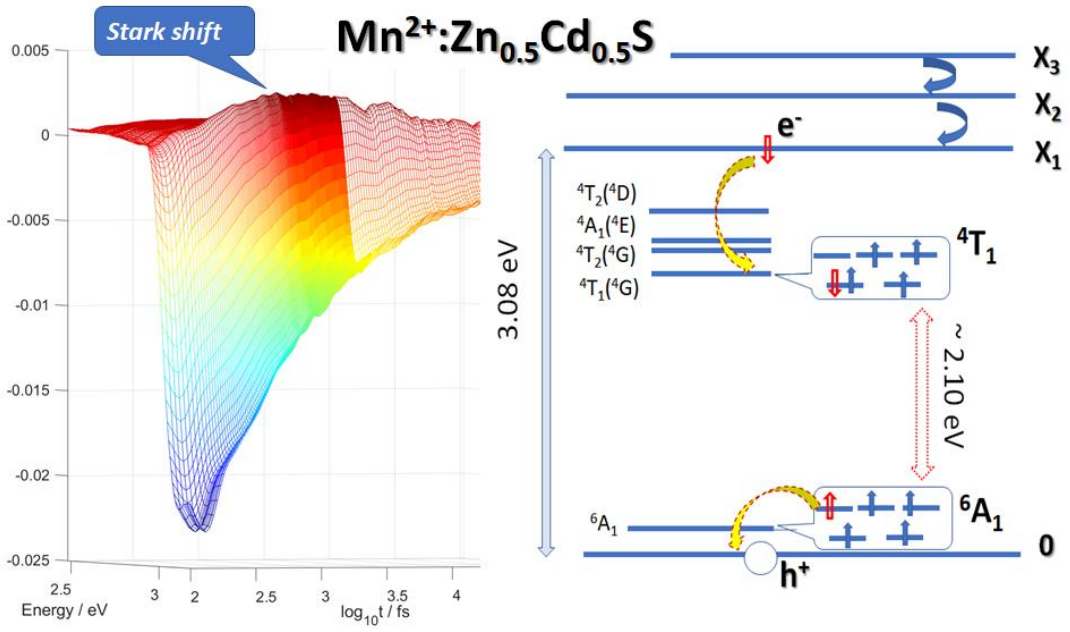

Fig.1 Femtosecond transient absorption spectra of Mn^{2+}:$Zn_{0.5}Cd_{0.5}S$/ZnS QDs (left). Stark peak evidences the charge transfer. Scheme of charge transfer events leading to the Mn^{2+*} excitation (right).

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 $Mn^{2+}(d^5)$* 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: Silicon electronics at atomic and molecular scales

Daniel Moraru[1]

[1]*Research Institute of Electronics, Shizuoka University, Hamamatsu, Japan*

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.

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[3] D. Moraru et al, Nano. Res. Lett. 10, 377 (2015).
[4] G. Prabhudesai et al, Appl. Phys. Lett. 114, 243502 (2019).

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

V. Toma[1], A. Onaciu[1,3], C. Moldovan[1,3], G. Stiufiuc[2], C. M. Lucaciu[3], R. I. Stiufiuc[1,3]

[1]MedFUTURE Research Center for Advanced Medicine, University of Medicine and Pharmacy, Cluj-Napoca, Romania
[2]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania
[3]Faculty of Pharmacy, University of Medicine and Pharmacy, Cluj-Napoca, Romania

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 infra-red 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].

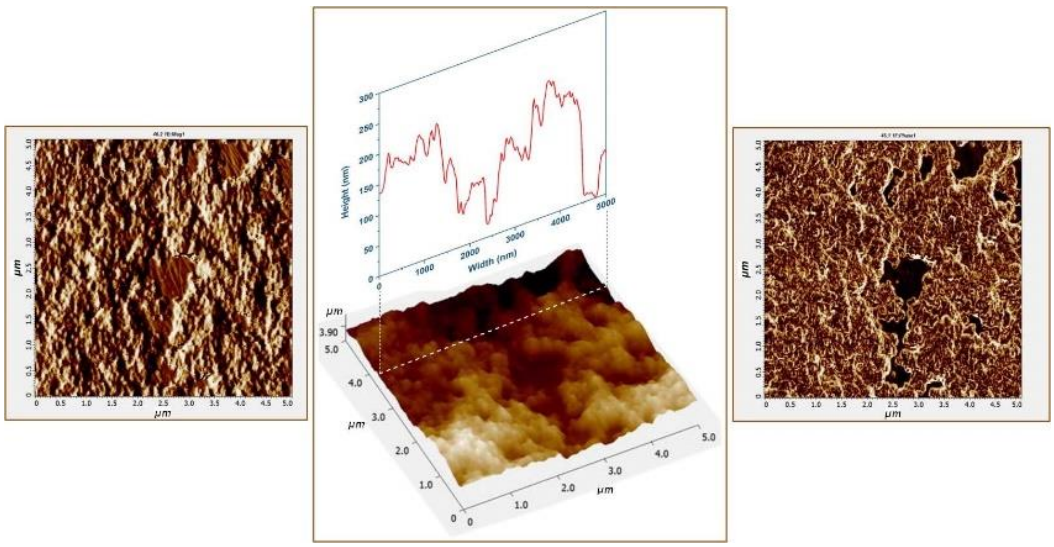

Fig.1. AFM image of the plamonic substrate

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.

[1] G.F. Stiufiuc et al., Nanomaterials (Basel), 10 (6) (2020) [2] C. Tefas, R. Stiufiuc et al., Analytical and bioanalytical chemistry, 413 (2021)

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

Valentina Dinca[1]

[1]*FOTOPLASMAT center, NILPRP, Magurele, Romania*

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.

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

L. Hrostea[1], L. Leontie[2], M. Girtan[3]

[1]Research Center on Advanced Materials and Technologies (RAMTECH), Department of Exact and Natural Sciences, Institute of Interdisciplinary Research, Alexandru Ioan Cuza University of Iasi, Iasi, Romania
[2]Faculty of Physics, Alexandru Ioan Cuza University of Iasi, Iasi, Romania
[3]Photonics Laboratory, (LPhiA), Faculty of Sciences, Angers University, Angers, France

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 Lectures

Hall 2

Online

PAMS-IL: Materials Design: How to choose dopants suitable for achieving tailored functional oxide films

T. Yamamoto[1]

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

We have been developing a technology which enables high film-deposition-rate such as 170 nm/min, 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. The TCO films are based from *n*-type doped ZnO- and In_2O_3-based films.[1-4] We

have been choosing several types of dopants suitable for achieving oxide films that meet the properties and functionals specific applications require [1]. For achieving reliable solid devices, the use of dopants that have high oxygen affinity compared with host metal atoms is essential. For example, for In_2O_3 films, W and Ce atoms have advantages over the conventional Sn atoms. This leads to supressment of the generation of oxygen vacancies in the vicinity of the substitutional-type dopant sites. On the other hand, note that ionic radii of dopant metal atoms which strongly depend on their charge states and on the coordination numbers play a critical role in controlling the residual strain in doped films.[1] Recently, we reported Ce- and H-codoped In_2O_3 films (ICO:H)

with a thickness of 100 nm showing high Hall mobility of 145 $cm^2/(Vs)$. [1,2] Incorporating ICO:H-based electrodes instead of Sn-doped In_2O_3-based electrodes improved the performance of Si heterojunction solar cells.[2] In addition, we achieve that 5-nm- and 30-nm-thick W-doped In_2O_3 films show Hall mobility of 57.7 and 97.4 $cm^2/(Vs)$, respectively.[3]

Fig. 1. Comparison of images of 20-inch LCD TV with GZO- and ITO-based electrodes. The fabrication were conducted by Sharp Co., Ltd.

Concerning ZnO films that have advantage of high optical visible transparency over In_2O_3 films, Al and Ga atoms having high O affinity as substitutional-type dopants have been reported. In previous work, we succeeded in the fabrication of liquid crystal displays with Ga-doped ZnO-based (GZO) electrodes produced with the conventional production lines (Fig. 1).[4]. It is easy to realize high carrier concentration GZO films exhibiting heat resistance. Note that Ti-doped ZnO films show excellent performance of the heat resistance. We discuss how to choose the dopants meeting application requirements from theoretical and experimental viewpoints.

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[3] Y. Furubayashi, M. Maehara, and T. Yamamoto, J. Phys. D: Appl. Phys. 53 (2020) pp. 375103-1-375103-7 (7 pp).
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PAMS-IL: Measurements of single-electron tunneling through atoms in nanoscale devices

D. Moraru[1]

[1]*Research Institute of Electronics, Shizuoka University, Japan*

Silicon electronics is the foundation of the accelerated progress in computation power and performance of recent decades, following the Moore's law of device (transistor or diode) miniaturization. In this lecture, this trend and implications for

the foreseeable future will be first described, as we are entering a regime of dimensionality well below 10 nm.

In this regime and beyond, dopants (impurities) randomly located inside or near the active region of the devices can have dramatic effects on the electron transport. Although this is generally considered detrimental for conventional electronics, it will be shown how such effects can be harnessed to provide proof-of-concept demonstrations of quantum-mechanical tunneling (even down to single-electron tunneling level) through atomic structures embedded in Si nanodevices [1].

We will explain how single-electron tunneling (SET) works and how to measure SET transport via individual donors [2-4] or via clusters of donors [5-8] working as quantum dots, not only in transistors, but also in tunnel diodes [9]. The lecture will present not only the key results, but also the critical points of the technology for achieving such accurate, low-level measurements of transport through atoms in nanoscale devices.

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[3] E. Hamid, D. Moraru *et al*., Phys. Rev. B **87**, 085420 (2013).
[4] A. Samanta, D. Moraru, T. Mizuno, and M. Tabe, Sci. Rep. **5**, 17377 (2015).
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[7] A. Samanta, D. Moraru *et al*., Appl. Phys. Lett. **110**, 093107 (2017).
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PAMS-IL: Characterisation of solids with the (Scanning) Transmission Electron Microscope

Jörg K.N. Lindner[1,2,3]

[1]Nanopatterning-Nanoanalysis-Photonic Materials Group, Department of Physics, Paderborn University, Paderborn, Germany,
email: lindner@physik.upb.de
[2]Centre for Optoelectronics and Photnics Paderborn, Paderborn, Germany
[3]Institute for Lightweight Design with Hybrid Systems, Paderborn, Germany

State-of-the-art (scanning) transmission electron microscopy (S)TEM today allows for a characterization of solid materials at an unprecedented spatial and energy resolution (Fig. 1). While the time and effort to be payed often exceeds by far the investmens of other techniques, (S)TEM frequently delivers the answers to questions left open by other analytical techniques.

In this presentation, an overview will be given on the fundamental concepts of (S)TEM microscopy and related spectroscopical techniques which exploit either the characteristic X-rays generated by impinging electrons (Energy Dispersive X-ray spectroscopy EDX/EDS) or the specific electron energy losses and gains due to inelastic electron solid interactions (Electron Energy Loss/Gain Spectroscopy EELS/EEGS).

Image formation in TEM and STEM will be explained on the basis of fundamental electron-solid interactions, emphasizing factors which have an impact on the interpretation of contrasts obtained. Examples will be given for the successful application of EDX and EELS techniques to reveal the local chemical nature of crystalline layer structures, the measurement of local

phonons and plasmons by EEGS and EELS in nanostructures as well as the analysis of internal magnetic and electric fields by differential phase contrast (DPC) STEM, the latter ones with even subatomic resolution. The aim is to provide an insight into the possibilities and possible pitfalls of modern (analytical) TEM/STEM techniques.

Fig. 1. Analyical (scanning) transmission electron microscope at Paderborn University.

Tuesday, September 28, 2021

08:00	**Invited and Oral Session** HALL-1
09:45	**Poster Session** Online
10:30	Coffee Break
11:00	**Invited Lectures** HALL-2
11:00	**Invited and Oral Session** Online
13:30	Lunch
15:00	**Plenary Session** Online
18:00	**Coffee Break and Poster Session** HALL 1
20:30	Dinner

HALL 1

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

S. R. Tripathi[1], K. Hashimoto[1], K. Yamamura[1]

[1]Department of Mechanical Engineering, Shizuoka University, Hamamatsu, 432-8541 Japan

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 (λ = 780nm, repetation rage = 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.

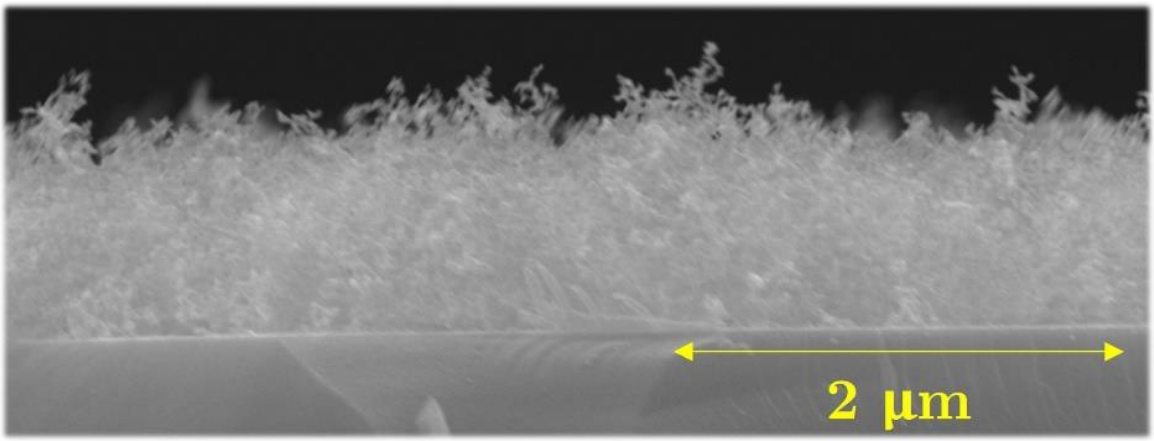
T5-O: Nanostructured metals as active layers for gas sensors

M. Hruška[1], J. Kejzlar[1], J. Otta[1], S. Havlova[1], P. Fitl[1], J. Vlcek[1], M. Novotný[2], Martin Vrňata[1],

[1]*Department of Physics and Measurements, University of Chemistry and Technology, Prague, Prague, Czech Republic*
[2]*Department of Analysis of Functional Materials, Institute of Physics of the Czech Academy of Sciences, Prague,* Czech Republic

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 phodetectors and sensing applications

D. Cristea[1], P. Obreja[1], R. Tomescu[1]

[1]Micro and Nano-Photonics, National Institute for Research and Development in Microtechnologies- IMT Bucharest, Romania

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.

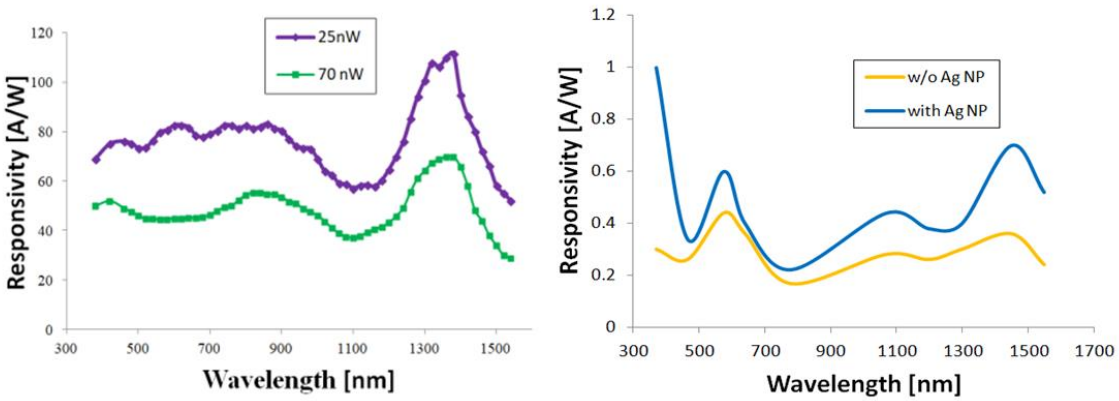


Fig. 1. Spectral responsivities for: a) hybrid photodetector PbS QDs/Si; b) ZnO NW- PbS:P3HT:PCBM ternary blend photodetector with and without Ag NPs.

We focused on solution processable materials based on quantum dots (QDs), nanowires and/or reduced grapheme 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

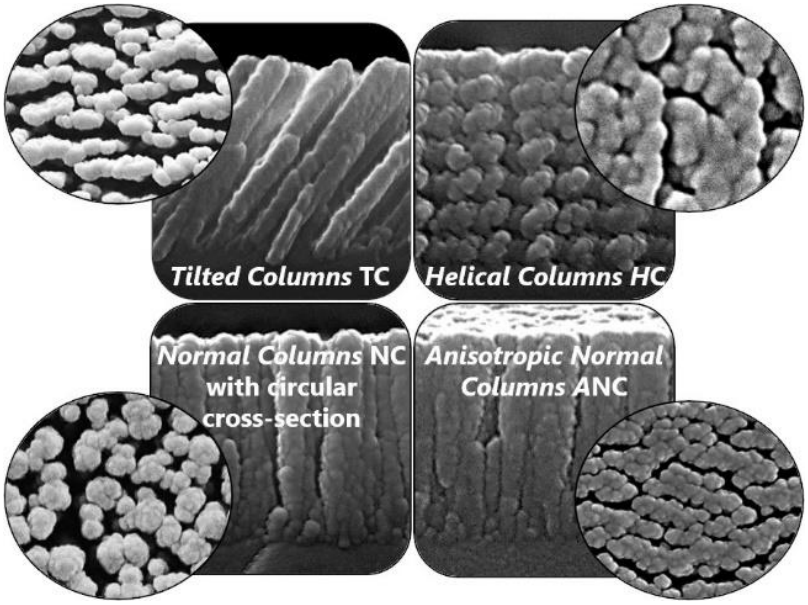
C. Marsal[1], E. Panchout[1], B. Giroire[1], C. Dupeyrat[2], T. Girardeau[1], F. Paumier[1]

[1]Institut Pprime, CNRS - Université de Poitiers - ISAE-ENSMA - UPR, Poitiers, France
[2]Couches minces, Optronique, Safran Electronics & Defense, Saint-Benoît, France

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 TiO_2 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.

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[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

M.-A. Guerboukha[1], V. Gadenne[1], H. Mrezguia[2], L. Giovanelli[2], Y. Ksari[2], V. Jeux[3], G. Monier[4], J.-M. Raimundo[5], L. Patrone[1]

[1] Aix Marseille Univ., Université de Toulon, CNRS, IM2NP UMR 7334, Yncréa Méditerranée, ISEN Toulon, France
[2] Aix Marseille Univ., Université de Toulon, CNRS, IM2NP UMR, Marseille, France
[3] ESCOM Chimie, Compiègne, France
[4] Univ Clermont Auvergne, CNRS, SIGMA Clermont, Inst Pascal, F-63000 Clermont Ferrand, France
[5] CINaM UMR CNRS 7325, Aix-Marseille Université, France

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.

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Poster Session

Online

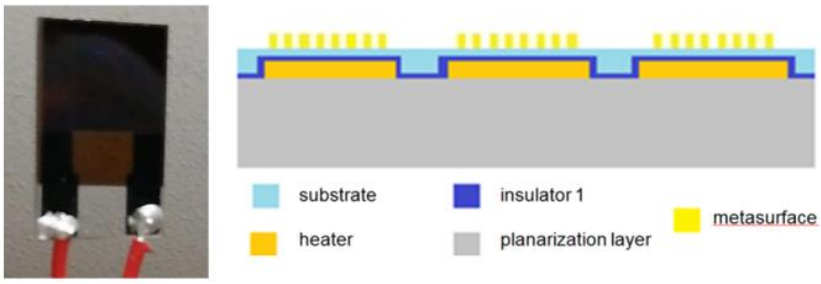
PAMS 4-P: Metasurface for sensing appications

R. Tomescu[1], V. Anastasoaie[1], C. Parvulescu[1], L. Mihai[2], C. Paun[1], D. Cristea[1]

[1]National Institute for Research and Development in Microtechnology – IMT Bucharest, 126A, Erou Iancu Nicolae Street, 077190, Voluntari, Ilfov, Romania
[2] Center for Advanced Laser Technologies – CETAL, National Institute for Laser Plasma and Radiation Physics, Magurele, Romania

We propose a compact photonic device that presents an improved and controlled emissivity on specific mid-nfrared domain which can be succesfuly used in sensing appications. Furthermore, we demonstrate that the device can be used to investigate the high levels of CO_2 that maiy accumulate in an infrastructure, or in capnography applications [1].
The device that acts as a narrowband IR emitter is composed of a metal-dielectric-metal (MDM) metasurface with controlled spectral emissivity/absorptivity achieved with geometrically

tuned electromagnetic resonances, and a broad-band IR source (a heater) - fig. 1. The structure operates on the Kirchhoff's law on thermal radiation which states that any heated absorber can emit thermal radiation at the same wavelength as the one absorbed. The MDM metasurface for the IR perfect absorbers/emitters consist in an array of sub-wavelength plasmonic structures, an insulator and a metal layer acting as a back-plane [2].



a) b)

Fig. 1 Integrated narrow-band IR emmiter based on metasurfaces: a) fabricated structure; b) cross-section

Table 1 Metasurface for CO2 sensing applications

Sample	Metasurface parameters		Micro-heater parameters		Emision spectral domaine
	D [μm]	P [μm]	No. menaders	Pads type	
A11	1	3	3	wide	3.8....4.3
A5	1.2	3	2	narrow	3.9...4.35
A4	1.4	4	3	narrow	4.2....4.6
A18	1.6	3	2	wide	3.8....4.3
B16	2.1	3	3	wide	4.25...4.5
B4	2.2	4	3	narrow	4.25...4.55
B17	2.2	4	2	wide	4.25...4.5

The main aim was the integration of a micro-heater with a specifically tailored metasurfaces structure. The heater is used as a broad-band IR source and also as a back-reflector for the matasurface-based absorber/emmiter to simplify the technology process. It is composed of 80 nm thick platinum layer in meander configuration. The resistor area is 1 cm^2. The

metasurface structure patterned on top of thermal source consists of an array of gold circular-shaped resonators with diameter (D) in the order of micrometres, configured to improve the light absorption within a narrow band interval in the IR domain.

Four types of micro-heaters have been designed, simulated, fabricated and characterized: narrow or wide pads; two or three meanders [3]. The metasurface parameters where specifically designed in order to obtain an absorption maximum placed in the spectral absorbtion interval of CO_2. In table 1 are presented several structures that offer de possibility of detecting CO_2. To characterize the device as an IR source a non-dispersive Infrared (NDIR) gas sensing system was built.

Acknowledgments. This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitalization, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PED-2019-1300, within PNCDI III.

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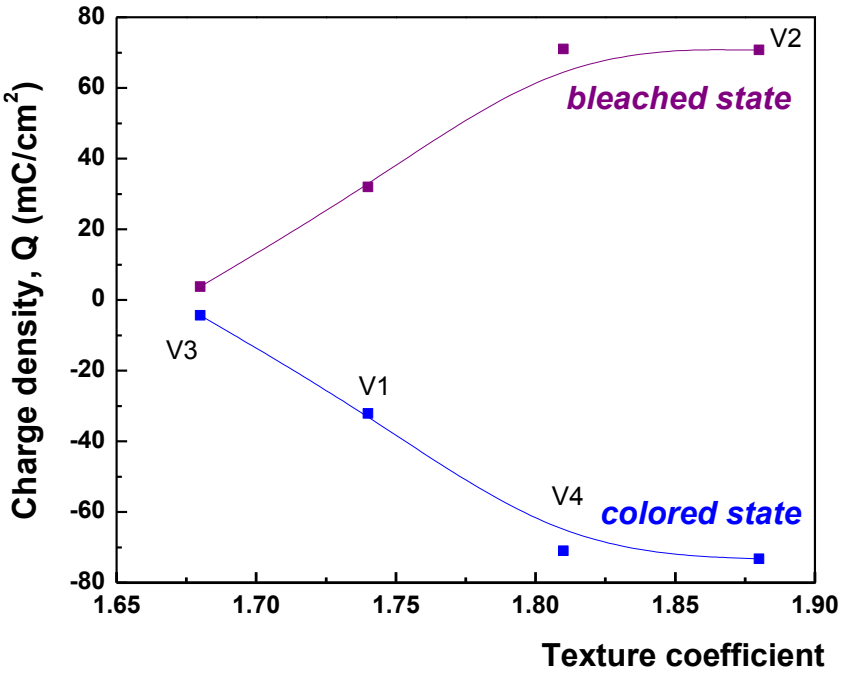
PAMS-P: Orthorombic V_2O_5 for electrochromism and charge storage devices: unveiling the microstructural features via non-destructive methods

C. Romanitan[1], I.V. Tudose[2,5,6], K. Mouratis[2,4], M. Popescu[1], C. Pachiu[1], S. Couris[7] E. Koudoumas[2,3], M. Suchea[1,2]

[1]National Institute for Research and Development in Microtechnologies, Romania

[2]*Center of Materials Technology and Photonics, School of Engineering, Hellenic Mediterranean University, Heraklion, Greece*
[3]*Department of Electrical and Computer Engineering, School of Engineering, Hellenic Mediterranean University, Heraklion Greece*
[4]*Physics Department, University of Patras, 26500 Patras, Greece*
[5]*Chemistry Department, University of Crete, Heraklion, Greece*
[6]*Institute of Electronic Structure and Laser, Foundation for Research & Technology-Hellas, Heraklion, Crete, Greece*
[7]*Physics Department, University of Patras, Greecce*

It is well known that the materials to be used for electrochromic applications must fulfill many of the same criteria as battery electrodes and they must be able to react very fast with small cations such as hydrogen or lithium and totally reversibly [1,2].



[4]

[5] Fig. 1. The dependence of the charge density of bleaching and coloring with the texture coefficient of layered V_2O_5

Vanadium oxides have gained a constantly growing interest in this field, because of their varying material properties according to oxidation state. We report a study based on the texture coefficient and electrochromism that unveils the

relationship between the texture coefficient on (001), i.e. the alignment of the atomic planes along the z-direction and the inserted charge storage on coloration and bleaching in nanostructured orthorhombic vanadium pentoxide obtained by spray pyrolysis technique – Fig. 1. We start from our encouranging previous results in V_2O_5 regarding the crystalline structure [3,4].

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PAMS-P: Structural and morphological proprieties of core-shell $CoFe_2O_4$@SiO_2@Au nanoparticles

A. Szatmari[1], R. Bortnic[1], R. Hirian[1,2], G. Souca[1], R. Dudric[1], V. Vinterel[1], V. Toma[2], R. Stiufiuc[2], E. Burzo[1], R.Tetean[1]

[1]Faculty of Physics, Babes-Bolyai University, Cluj Napoca, Romania
[2]Department of Bionanoscopy, MedFuture Research Center for Advance Medicine, "Iuliu Hatieganu" University of Medicine and Pharmacy, Cluj Napoca, Romania

Core-shell $CoFe_2O_4$@SiO_2@Au nanoparticles have been successfully synthesized through the Polyvinylpyrrolidone (PVP) assisted hydrothermal method ($CoFe_2O_4$ – core) followed by a two-step wet chemical deposition (first SiO_2 followed by Au – shell). Synthesis of the core particles were carried out in a sealed off 100 ml PPL Lined Hydrothermal Autoclave using

Ehylene glycol as solvent. The addition of PVP to the synthesis was proven to restrict agglomeration of the as obtained particles. X-Ray Diffraction pattern reveal the presence of single phase $CoFe_2O_4$ particles. The average crystallite size given by using the Debye-Scherrer equation was calculated to be 19 ±1 nm. Transmission electron microcopy (TEM) images reveal the formation of "raspberry-like" spherical $CoFe_2O_4$ core particles with an average particle size of 64 nm. The SiO_2@Au shell was then obtained through a two-step chemical deposition on the functionalized core particles. In both cases, (deposition of SiO_2 and of Au) (3-Aminopropyltriethoxysilane was used as a functionalization agent, although different mechanisms of deposition were employed. A variation of the Stöber method was used in order to grow the SiO_2 layer while the gold shell was formed by reducing Au from $HAuCl_3$ and growing it on the positively charged functionalized core. 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.

PAMS-IL: X-ray generation using pyroelectric crystals excited by laser light

H. Mimura[1], T. Ishida[1], T. Masuzawa[1], N. Yoichiro[1], T. Aoki[1]

[1]*Shizuoka University, Research Institute of Electronics, Hamamatsu, Japan*

Pyroelectric crystals such as lithium niobate ($LiNbO_3$) and lithium tantalite ($LiTaO_3$) have spontaneous polarization which varies with temperature. The surface polarization charge of the crystal is usually screened by the free charges that accumulate on the surface at equilibrium. The change in polarization of the crystal due to the temperature change generates a high electric field, emitting energetic electrons without external voltage when heated or cooled. [1] X-ray sources [1] have been reported as applications of the electron emission from pyroelectric crystals. One of the X-ray sources using a pyroelectric crystal excited by a Peltier device is commercialized. The use of a Peltier device, however, has problems. It requires an electric wire, the response is slow due to its heat capacity, and downsizing is difficult. To remove a Peltier device, Nakahama et al. irradiated an contentious infrared laser (CW Nd:YLF) on the graphite layer. [2] However, in X-ray sources using an IR laser, the response is also slow, because it takes a time that the temperature of the crystal rises up. In this paper, we have excited a $LiNbO_3$ crystal with a pulse UV laser light (the wavelength of 266 nm) in the vacuum. Electrons emitted from the $LiNbO_3$ crystal collided with a Cu target and generated X-ray.

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PAMS-IL: Emission and detection of terahertz waves and their industrial and biomedical applications

S. R. Tripathi[1] and T. Kawauchi[1]

[1]Department of Mechanical Engineering, Shizuoka University, Hamamatsu, 432-8561 Japan

The electromagnetic waves with the frequency range spanning from few hundreds of gigahertz (GHz) to few terahertz (THz) are known as terahertz waves (1 THz = 10^{12} Hz = 300 μm = 4.1 meV). These waves can penetrate through wide variety of materials such as plastics, papers and cloths making them an alternative to X-rays in many applications such as security screening and non-destructive testing and evaluation. Moreover, wide variety of materials such as narcotics and explosives possess a spectral fingerprint in THz frequency region making them detectable based on THz spectral imaging. Along with these applications, sub-terahertz waves are being exploited in wireless networks for 6G communication owing to their ability to satisfy the increasing demand for high-speed data transfer. All these characteristics make the THz wave an attractive option in diverse fields from biomedical sciences and homeland security to information and communication technologies. In this presentation, I will briefly explain the emission and detection of terahertz waves using photoconductive antenna and non-linear optical crystals. Particularly, I will introduce high power terahertz wave generation using non-linear optical crystal via optical rectification of femtosecond pulse. At the end of the

presentation, and I will introduce few industrial applications of 2D and 3D terahertz wave imaging for non-destructive testing and evaluation. Besides this, recent results of biomedical applications of terahertz waves will also be presented.

PAMS-IL: Creating Electrical Current Bistability in Nanocomposites

Shashi Paul[1]

[1]Emerging Technologies Research Centre, De Montfort University, Leicester LE1 9BH, United Kingdom

Over the last one decade, there has been a growing interest in the field of two terminal polymer memory devices as a low-cost, easily manufacturable alternative to conventional silicon memory technologies. Several possible device structures and materials have been proposed in literature, most of them consisting of a blend nanomaterial(s) and insulating matrix – such blend is called nanocomposite. The nanocomposite layer is sandwiched between top and bottom metal contacts. The memory effect has also been demonstrated on the nano-scale, opening up the possibility of having cheap, high density memory devices capable of competing with today's silicon technologies. While all the reported studies have been conducted on similar memory structures, there is still much discussion over the physical mechanisms responsible for the memory effect. This proposed talk will discuss the recent development on understanding the bistability, based on internal electric field, in nanocomposite memory devices and the obvious benefits of implementing nano-particles for this

purpose and move on to expound upon the problems associated with such devices.

Plenary Session

Online

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

Ortwin Hess[1,2]

[1]*School of Physics and CRANN Institute, Trinity College Dublin, Ireland*
[2] *The Blackett Laboratory, Imperial College London, UK*

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

Simion Astilean[1,2]

[1]*Department of Bimolecular Physics, Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania*

[2]*Nanobiophotonics and Laser Microspectroscopy Center, Interdisciplinary Research Institute in Bio-Nano-Sciences, Babes-Bolyai University, Cluj-Napoca, Romania*

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 nanoprobes, 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 phothotermal 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.

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

Jörg K.N. Lindner[1,2,3]

[1]Nanopatterning-Nanoanalysis-Photonic Materials Group, Department of Physics, Paderborn University, Paderborn, Germany,
[2]Centre for Optoelectronics and Photnics Paderborn, Paderborn, Germany
[3]Institute for Lightweight Design with Hybrid Systems, Paderborn, Germany

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 mirophase 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 paiving the way for applying BCP lithography for a big variety of nanopatterning tasks.

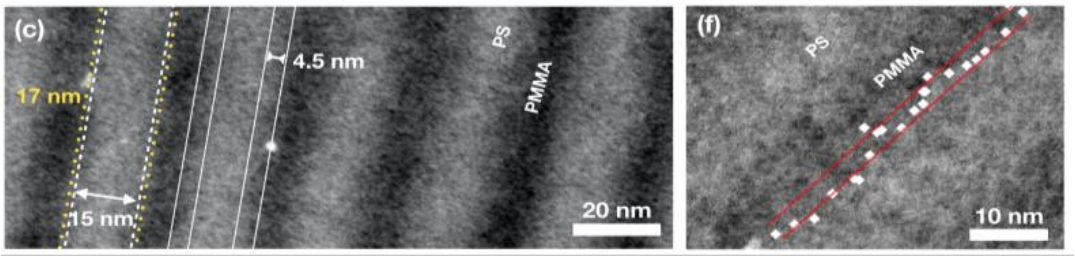

Fig. 1. STEM-ADF images of a lamellar PS-b-PMMA BCP film. [1]

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T1-PL: Silicon: Past, present and future

Shashi Paul[1]

[1]Emerging Technologies Research Centre, De Montfort University, Leicester LE1 9BH, United Kingdom

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.

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

D. Duca[1], C. Pirim[1], M. Vojkovic[1], Y. Carpentier[1], A. Faccinetto[2], M. Ziskind[1], C. Preda[3], C. Focsa[1]

[1]Université de Lille, CNRS, UMR 8523 - PhLAM - Physique des Lasers, Atomes et Molécules, Lille F-59000, France
[2] Université de Lille, CNRS, UMR 8522 - PC2A - Physicochimie des Processus de Combustion et de l'Atmosphère, Lille F-59000, France

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 (~200 µm 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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[3] A. Faccinetto, P. Desgroux, M. Ziskind, E. Therssen, C. Focsa (2011) Combust. Flame 158, 227-239.
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PAMS-4 Poster Session & Cofee Break

HALL 1

PAMS-P: Neutron reflectometry in applied research of interfaces with liquid and soft media at the IBR-2 reactor

Ye.N.Kosiachkin[1,2,4], M.V. Avdeev[1], V.I. Petrenko[1,2], V.I. Bodnarchuk[1], I.V. Gapon[1,2], O.V. Tomchuk[1,2], T.V. Tropin[1], A.V. Nagornyi[1,2], L.A. Bulavin[2] and V.L. Aksenov[3,1]

[1]Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia
[2]Physics Department, Taras Shevchenko National University of Kyiv, Ukraine
[3]National Research Centre 'Kurchatov Institute', Moscow, Russia
[4]Institute for Scintillation Materials, Kharkiv, Ukraine

Nowadays studies on the free surface of liquids, soft condensed matter interfaces, as well as on hidden interlayers are widely in demand for a huge variety of branches of science. Therefore, the development and improvement of neutron reflectometers with a horizontal sample plane are of current

interest. GRAINS neutron reflectometer [1] is a user program facility situated at the IBR-2 pulsed reactor (JINR, Dubna). The reflectometer operates in the time-of-flight mode (with a wavelength range of 0.05 – 1nm) taking advantage of a broad wavelength band of the cold moderator at the IBR-2. The inclined incident beam of thermal neutrons (grazing angle of 3 – 25 mrad, flux at the sample of 2×10^6 $s^{-1}cm^{-2}$) is formed by special deflecting neutron mirrors. This work presents the results of experiments carried out on the GRAINS reflectometer and demonstrate applicability of the neutron reflectometry method realized on the facility in nanoparticles and polymer layers, electrochemical interfaces, biological, etc. studies

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PAMS-PAndreev conductance through a quantum dot-Majorana ring structure

L. Máthé[1,2], D. Sticlet[1], L. P. Zarbo[1],

[1]Center of Advanced Research and Technologies for Alternative Energies (CETATEA), National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
[2]Department of Solid State Physics and Advanced Technology, Faculty of Physics, Babeș-Bolyai University, Cluj-Napoca, Romania

We study electron transport, in the presence of local and crossed Andreev reflection processes, in a quantum dot coupled to Majorana bound states located at the ends of a topological superconductor nanowire. A measurable electric current passes

through the quantum dot due to its coupling to two normal leads. The dot-Majorana system forms a ring structure which is threaded by a magnetic flux. The tunable magnetic flux allows one to manipulate the local and nonlocal processes. We use the nonequilibrium Green's function formalism to derive the current formulas and apply the equation of motion technique to determine the relevant retarded Green's functions. The influence of magnetic flux, dot energy level, dot-Majorana and dot-lead couplings on linear and differential conductances of electron, local Andreev and crossed Andreev reflection processes are discussed in detail at zero and finite temperatures.

PAMS-P: Hematite and cobalt ferrite nanostructures isolated in MCM-41

L. Popa[1], M. Ignat[2], E. Ware[3], A. Popa[4], D. Toloman[4], F. Iacomi

[1]*Faculty of Physics, Alexandru Ioan Cuza University, Iasi, Romania*
[2]*Faculty of Chemistry, Alexandru Ioan Cuza University, Iasi, Romania*
[3]*Faculty of Engineering, Imperial College London, U.K.*
[43]*National Institute for Research and Development of Isotopic and Molecular Technologies Cluj-Napoca, Romania*

Magneticc compounds like hematite and cobalt ferrite, were isolated in a highly ordered mesoporous material, MCM-41, with a quasi-one-dimensional array. MCM-41 has a topology of regular hexagonal parallel channels with diameters of 2-3 nm. The MCM-41 nanopowder was synthesized by using an amino-functionalized conventional method and the nanocomposites were obtained by wet impregnation. Phase composition and

morphology of the products were investigated by XRD, SEM/EDS, TEM, FTIR, BET and EPR techniques and the obtained results confirmed the formation of hematite and cobalt ferrite nanostructures in the MCM-41 channels.

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

V. Vinteler[1], G. Souca[1], R. Hirian[1], S. Mican[1], R. Bortnic[1], R. Tetean[1]

[1]Solid State Physics and Advanced Technology, Babes-Bolyai University, Faculty of Physics, Cluj-Napoca, Romania

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 Gd_4Co_3 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 Tc=394-399K, close to 404 K, the $GdCo_2$ transition

temperature. Finally, the influence of titanium atoms substitution on cobalt site is discussed.

PAMS-P: Magnetic properties and magnetocaloric effect in $La_{0.7-x}Eu_xBa_{0.3}MnO_3$ compounds.

R. Atanasov[1], R. Hirian[1], R. Bortnic[1], G. Souca[1], F. Popa[2], E. Covaci[3], I. Deac[1]

[1]Faculty of Physics, Babes-bolyai University, Cluj-Napoca, Romania
[2]2 Department of Materials Science and Engineering, Technical University of Cluj-Napoca, Cluj-Napoca, Romania
[3]Faculty of Chemistry, Babes-Bolyai University, Cluj-Napoca, Romania

Structural, magnetic properties and magnetocaloric effect of $La_{0.7-x}Eu_x$ $Ba_{0.3}MnO_3$ 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.

Wednesday, September 29, 2021

08:00	**Plenary Session** HALL 1
10:20	Coffee Break
11:00	**Invited Lectures** HALL 2
13:35	Lunch
15:00	**Plenary Session** Online
18:00	Cofee Break
18:30	**Plenary&Invited & Oral Session**
20:35	Gala Dinner

Hall-1

T6-PL: Silicon-based quantum emitters at telecom frequency

M. Abbarchi[1]

[1]*NOVA Team-IM2NP - UMR CNRS 7334 Aix-Marseille Université, Faculté des Sciences de Saint Jérôme, Case 142 13397 Marseille Cedex 20*

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

H. Mimura[1,2], S. Sakakibara[1,2], Y. Neo[1]

[1]Shizuoka University, Research Institute of Electronics, Hamamatsu, Japan
[2]Hamamatsu 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.

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.

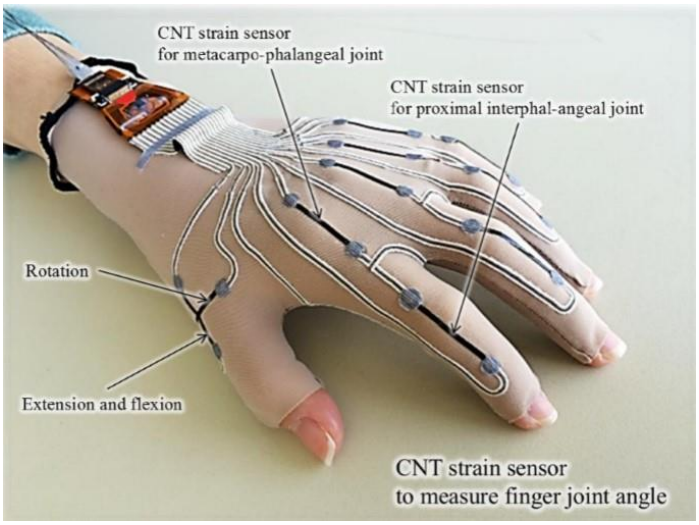

Fig.1 Data glove using the CNT strain sensors.

[1] Y. Inoue, K. Kakihata, Y. Hirano, T. Horie, A. Ishida, and H. Mimura, Appl. Phys. Lett. 92 (2008) 213113.
[2] K. Suzuki, K. Yataka, Y. Okuyama, S. Sakakibara, K. Sako, H. Mimura and Y. Inoue, ACS sensors (2016) 817.

T7-PL: Epitaxial ferroelectric HfO_2 films

Florencio Sanchez[1]

[1]*Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Spain, fsanchez@icmab.es*

Ferroelectric HfO_2 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 HfO_2 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 $Hf_{0.5}Zr_{0.5}O_2$ 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.

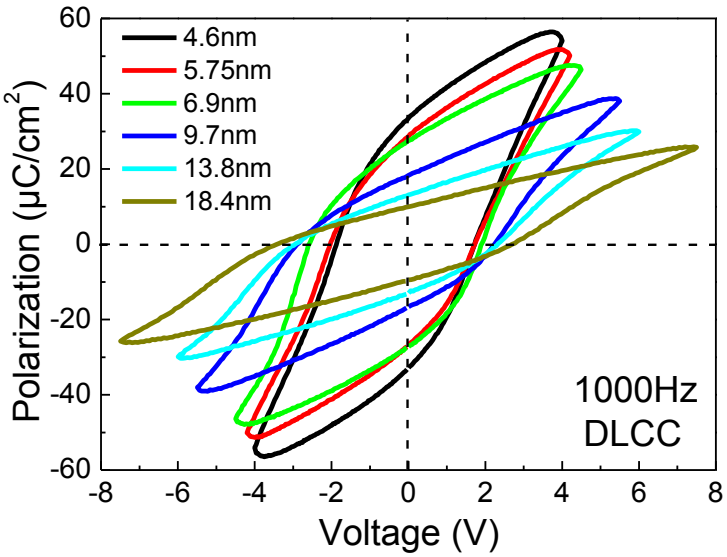

Fig. 1. Ferroelectric polarization loops of epitaxial $Hf_{0.5}Zr_{0.5}O_2$ films on Si(001). Films thinner than 5 nm show a remanent polarization above 30 $\mu C/cm^2$.

[1] I. Fina and F. Sánchez, Appl. Electron. Mater. 3, 1530 (2021)
[2] T. Song, S. Estandía, H. Tan, N. Dix, J. Gazquez, I. Fina, F. Sánchez, Adv. Electron. Mater. (2021, accepted)
[3] T. Song, R. Bachelet, G. Saint-Girons, N. Dix, I. Fina, and F. Sánchez, J. Mater. Chem. C (2021, accepted)
[4] T. Song, R. Bachelet, G. Saint-Girons, R. Solanas, I. Fina, and F. Sánchez, ACS Appl. Electron. Mater. 2, 3221 (2020).

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

J.-N. Aqua[1], K. R. Hannikainen[2], I. Berbezier[2], L. Favre[2], A. Ronda[2]

[1]*INSP, Sorbonne Université/CNRS, Paris, France*
[2]*IM2NP, Aix Marseille Université/CNRS, Marseille, France,*

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].

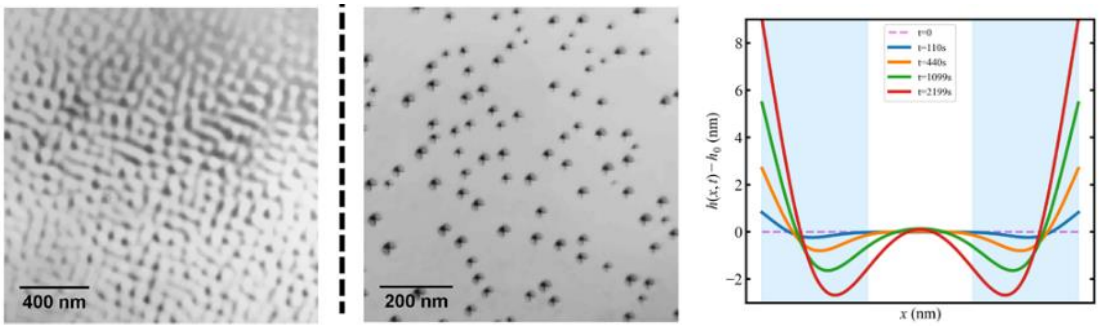

Fig. 1. (Left) TEM images of SiGe films deposited on Si(001) with a mean Ge composition of 0.3 (left) and 1 (right) ; (Right) Theoretical evolution of a strained mesa near its free boundaries.

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.

[1] J.-N. Aqua, I. Berbezier, L. Favre, T. Frisch, A. Ronda, *Physics Reports* 522 (2013) 59.
[2] K. Liu, I. Berbezier, L. Favre, A. Ronda, M. Abbarchi, P. Donnadieu, P. W. Voorhees and J.-N. Aqua, *Nanoscale,* **11** (2019) 7798
[3] K. Liu, I. Berbezier, T. David, L. Favre, A. Ronda, M. Abbarchi, P. W. Voorhees, J.-N. Aqua, *Physical Review Materials* **1** (2017) 053402
[4] K. R. Hannikainen, L. Favre, A. Ronda, I. Berbezier, D. Dutartre, J.-N Aqua, *to be published*.

Invited Lectures

HALL 2

PAMS-IL: Physics of Thermo-magneto-electric phenomena in liquids

A. Chiolerio[1]

[1]*Center for Converging Technologies, Istituto Italiano di Tecnologia, Genova, Italy*

Stemming out from the last three years research in the field of liquid state waste to heat power conversion, this lecture summarizes the most important physical relations to describe

a multi-phase colloidal system under non-equilibrium conditions, particularly, in the presence of an external magnetic field, a thermal gradient and a gravitational field. Fig. 1 shows the thermo-magneto-electric device operating at the liquid state and providing waste heat to power capabilities.

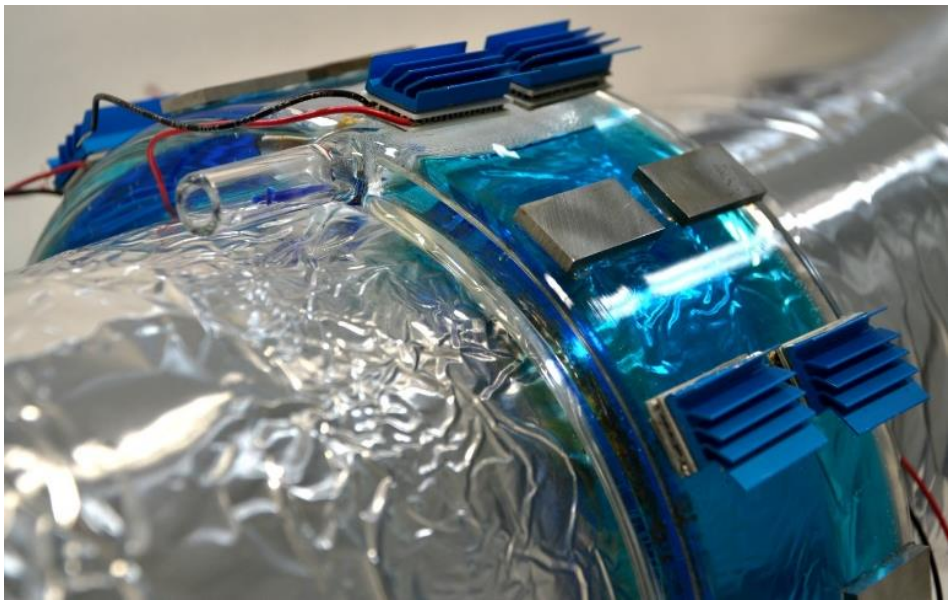

Fig. 1. Thermo-magneto-electric device providing waste heat to power capabilities.

Thermodiffusion equation, Navier - Stokes's momentum equation, Fourier heat equation are introduced.
A particular emphasys is given to magnetic fluids, where superparamagnetic nanoparticles are subjected to the magnetic volume force, whose expression is discussed considering the recent literature [1].
A few practical examples are given of mixed composition colloids, exploiting multi-physics effects that also involve pyroelectricity [2], triboelectricity [3] and the Ludwig-Sorét effect.

[1] L. Cecchini and A. Chiolerio, Journal of Physics D: Applied Physics. In press (2021) 10.1088/1361-6463/ac0a0a

[2] M. Bevione, E. Garofalo, L. Cecchini and A. Chiolerio, MRS Energy & Sustainability 7 (2020) E38.
[3] E. Garofalo, L. Cecchini, M. Bevione, A. Chiolerio, Nanomaterials 10:6 (2020) 1181.

PAMS-IL: Pulsed laser deposition

F. Sánchez[1]

[1]*Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Spain*

Pulsed laser deposition (PLD) is the most commonly used technique to grow complex oxides. PLD is considered simple, but a good understanding of laser ablation and the PLD technique are necessary to take advantage of their benefits and avoid film off-stoichiometry. In this lecture, after a brief overview of the main thin film deposition techniques, I will first describe the laser ablation process and the properties of the generated plasma.

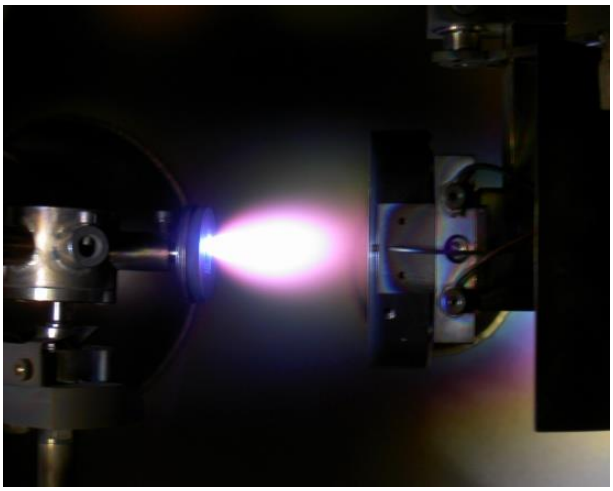

Fig. 1. Picture of a PLD plasma produced when an excimer laser beam ablates an oxide target (at the left of the image) under at oxygen atmosphere. The substrate heater can be seen at the right of the image.

Next, the main limitations and advantages of PLD will be discussed. Finally, the possibilities of in-situ control of epitaxial growth mechanisms when using in-situ reflection high-energy electron diffraction (RHEED) in PLD will be detailed.

PAMS-IL: Biophysical Perspectives of Membranes Through the Optics of Neutrons

Norbert Kučerka[1,2]

[1]*Frank Laboratory of Neutron Physics at Joint Institute for Nuclear Research in Dubna*
[2]*Faculty of Pharmacy at Comenius University in Bratislava*

The advances achieved over past decades developed to an extent that scattering approaches can successfully characterize the physical properties of disordered materials such as biomimetic membranes. The X-ray and neutron scattering methods are applied to elucidate the material properties previously thought to be the domain of other techniques, and even provide possibilities not present in any other methods. In particular, neutron diffraction is utilized to determine the distribution of water or individual components through deuterium labeling. Its ability to isolate individual molecular groups at the atomic level of detail is unique among biophysical techniques and is directly comparable to molecular model simulations. The advantage of the joint refinement of X-ray and neutron scattering measurements is reflected in the improved robustness of structural models employed and in increased details made available through these advanced models. The structural studies of lipid membranes and their changes due to the environmental and compositional changes represent an

important part of membrane biophysics that benefits in particular from the advancement of neutron scattering.

Plenary Session

Online

T6-PL: Tip-enhanced spectroscopies on 2-dimensional transition metal dichalcogenides and their interfaces

Dietrich R. T. Zahn[1]

[1]Semiconductor Physics, Chemnitz University of Technology, Chemnitz, Germany, zahn@physik.tu-chemnitz.de

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 CO_2 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.

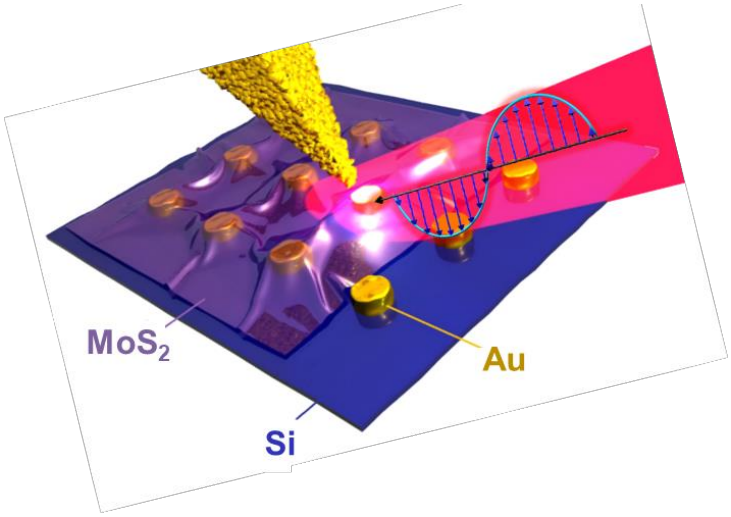

Fig. 1. Sketch of a TERS experiment investigating a MoS_2 monolayer deposited on an array of gold nanodisks on silicon. The gold tip of an atomic force microscope is tilted and the laser light focused onto the tip apex is polarized along the long tip axis for strong coupling to the localized surface plasmon resonance. The scattered light is collected by the same lens focusing the laser onto the tip.

In this contribution we deliver a short introduction to the most commonly used 2D semiconductors, namely the transition metal dichalcogenides (TMDCs), 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.

T4-PL: Multiscale analysis of perpendicular magnetic anisotropy and its electric field manipulation in spintronic devices

C. Tiusan[1,2,4], R. A. One[1,2], S. Mican[2], A. Mesaros[1], M. Joldos[1], H. Bea[3], L.D. Buda-Prejbeanu[3]

[1]*Technical University of Cluj-Napoca, Romania*
[2]*Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania*
[3]*Univ. Grenoble Alpes, CEA, CNRS, Grenoble INP, SPINTEC, 38000 Grenoble, France*
[4]*National Center of Scientific Research (CNRS) France*

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.

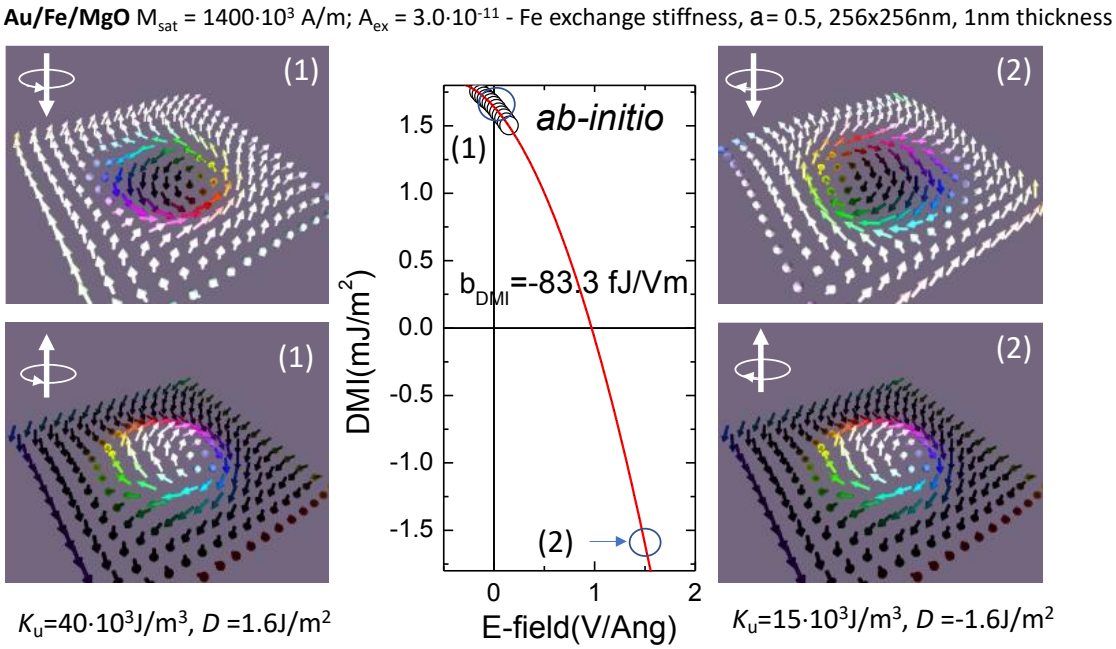

Fig.1 *Calculation of DMI dependence of electric field in Au/Fe/MgO(001) supercell. The gate controlled 4 state skyrmionic system: 2 chiralities + 2 core orientations) simulated by the mumax3 micromagnetic code* [4].

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.

[1] W-G. Wang, M. Li, S. Hageman, C.L. Chien, Nature Mater., vol. 11, pp. 64-68, 2012.

[2] Y. Shiota, T. Nozaki, F. Bonell, S. Murakami, T. Shinjo, Y. Suzuki, Nature Mater., vol. 11, pp. 39-43, 2012.
[3] P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G. K. H. Madsen and L. D. Marks, J. Chem. Phys., vol. 152, p. 074101, 2020.
[4] "The design and verification of mumax3", AIP Advances 4, 107133 (2014).

T4-PL: MAS NMR in advanced materials Investigations

R.V.F. Turcu[1,2]

[1]*National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj Napoca, Romania*
[2]*Faculty of Physics, Babes Bolyai University, Cluj Napoca, Romania*

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

A. Di Bartolomeo[1,2], E. Faella[1,2], F. Giubileo[2], A. Grillo[1,2], A. Pelella[1,2], M. Passacantando[3]

[1]Department of Physics "E. R. Caianiello", Univerisity of Salerno, 84084, Fisciano, Salerno, Italy
[2]CNR-Spin, 84084, Fisciano, Salerno, Italy
[3]Department of Physical and Chemical Science, University of L'Aquila, I-67100, Coppito, L'Aquila, Italy

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 MoS_2, WSe_2, $PdSe_2$, and $PtSe_2$. Nanosheets of TMDs, obtained by either mechanical exfoliation or chemical vapor deposition on SiO_2/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.

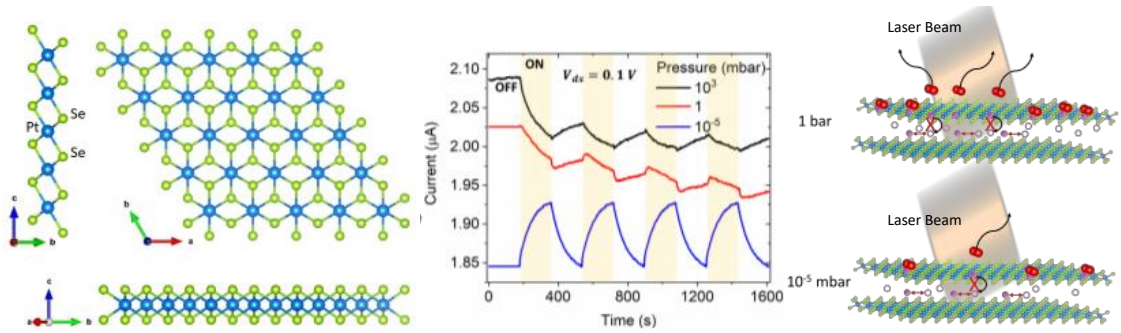

Fig. 1. (a) $PtSe_2$ structure. (b) Current in a $PtSe_2$ transistor at different pressures and under laser pulses, showing the coexistence of positive and negative photoconductivity. (c) Light-induced oxygen desoption in $PtSe_2$.

[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

N. Bityurin[1], A. A. Smirnov[1], A. Pikulin[1], A. Kudryashov[1]

[1]*Instutuite of Applied Physics RAS, Nizhny Novgorod, Russia,*

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.

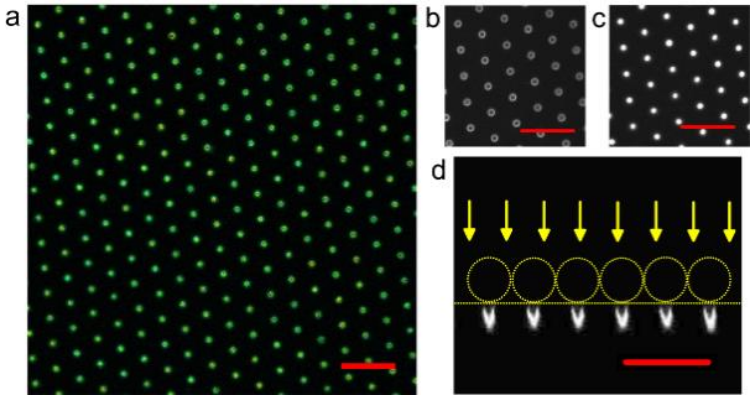

Fig. 1. Confocal microscope PL image of the periodic structure recorded by laser in photoinduced nanocimposite. [1]. Scale bar is 20 μm.

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.

Plenary, Invited and Oral Session

HALL 1

T13-O: Quantum transport through a quantum dot side-coupled to a Majorana bound state pair in presence of electron-phonon interaction

L. Máthé[1,2], D. Sticlet[1], L. P. Zarbo[1]

[1]*Center of Advanced Research and Technologies for Alternative Energies (CETATEA), National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania*
[2]Department of Solid State Physics and Advanced Technology, Faculty of Physics, Babeș-Bolyai University, Cluj-Napoca, Romania

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

Liviu Chioncel[1]

[1]*Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany*

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/ν_n, where Q is the transferred momentum and ν_n is the corresponding excitation energy.

Using the scaling variable Q_2/ν_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

Saikat Benarjee[1]

[1]*Physics of Condensed Matter and Complex Systems Group (T4), Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

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

Vladimir Dobrosavljevic [1]

[1] *Department of Physics and national High Magnetic Field Laboratory Florida State University, Tallahassee, USA*

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

Andreas Oestlin[1]

[1]*Theoretical Physics III, Center for Electronic Correlation and Magnetism, Institute for Physics, University of Augsburg, Germany*

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.

Thursday, September 30, 2021

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	Exccursion to Dali Museum

HALL 1

T9-PL: Interactions in the pre-AD mimicking model membranes

O. Ivankov[1,2], T. Murugova[1,2], T. Kondela[1,3], S. Kurakin[1,4], P. Hrubovcak[1,5], E. Ermakova[1], E. Dushanov[1,6], D. Badreeva[1], D. Soloviov[1,2], Kh. Kholmurodov[1,6], A. Kuklin[1,2], N. Kucerka[1,3]

[1]*Joint Institute for Nuclear Research, Dubna, Russia*
[2]*Moscow Institute of Physics and Technology, Dolgoprudny, Russia*
[3]*Comenius University in Bratislava, Bratislava, Slovakia*
[4]*Kazan Federal University, Kazan, Russia*
[5]*Šafarik University in Kosice, Kosice, Slovakia*
[6]*Dubna State University, Dubna, Russia*

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.

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T10-PL: Towards liquid state cybernetic systems

Alessandro Chiolerio[1]

[1]*Center for Converging Technologies, Istituto Italiano di Tecnologia, Genova, Italy*

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].

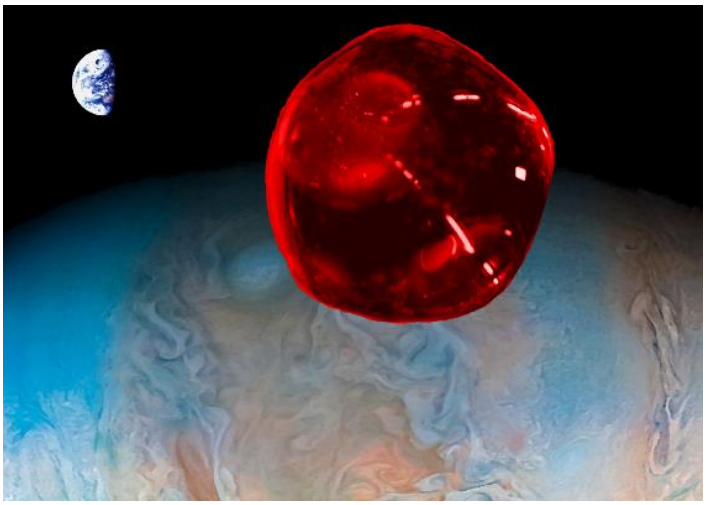

Fig. 1. Pictorial representation of a liquid state autonomous cybernetic system for space exploration. Not in scale are shown: Jupiter clouds (below), the Earth (top left), and the colloidal robot (in red).

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T1-PL: The device principle of low-dimensional high-gain phototransistors

Yaping Dan[1]

[1]*University of Michigan - Shanghai Jiao Tong University Joint Institute, Shanghai Jiao Tong University, Shanghai, China*

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.

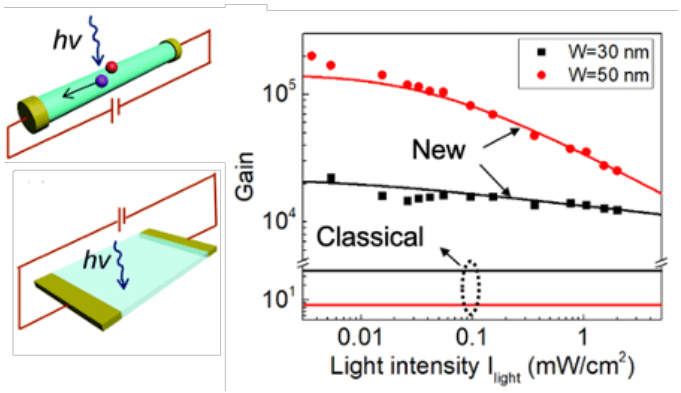

Fig.1. Explicit Gain Equations for Low Dimensional Phototransistors

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 (Fig.1). 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 phtoconductive devices and allow us to quantitatively design these in terms of photogain, bandwidth and dark current.

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T10-PL: Harmonic generation in random nonlinear crystals: application to ultrashort pulse characterization and analysis of domain statistics

Crina Cojocaru[1]

[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 trough 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. Nondestructibe 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.

Plenary and Invited session

Online

T13-PL: Floquet-Bogoliubov approach for time-periodic driven Luttinger liquids

Imke Schneider[1]

[1]*Theoretical Physics III, Institute for Physics, University of Augsburg, Germany*

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 Eriksson[1]

[1]*Department of Astronomy and Physics*
Uppsala University, Sweden

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 mulatiscale 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

Ioan M. Pop[1]

[1]*IQMT and PHI, Karlsruhe Institute of Technology, Germany, ioan.pop@kit.edu*

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.

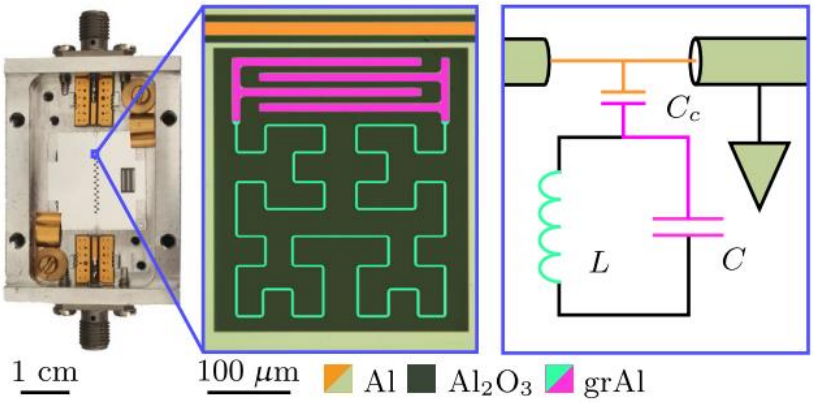

Fig. 1: Mo tectors (center), modeled as lumped element circuits (right) [1]

[1] F. Valenti et


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