7-10 July 2020

NN20

Book of Abstracts

A Warm Welcome to the NN20!

The **Intenational Conference on Nanosciences and Nanotechnologies (NN20)**, is the internationally established world-class event in Nanosciences and Nanotechnologies (N&N) that focuses on the latest advances on N&N and promotes profound scientific discussions between scientists and researchers and innovators from different disciplines.

The Program of the **17th year of the International Conference on Nanosciences & Nanotechnologies at 2-5 July 2020 in Thessaloniki** is a multidisciplinary collection of hot topics and a fine list of Invited Speakers related to the N&N fields, consisting of more than 80 Invited and 100 Oral presentations, 150 poster presentations and 15 running EU funded R&D Projects. These combined with the ISFOE International Symposium, the ISSON Summer Schools, the EXPO Exhibition and the B2B meetings that will take place in parallel within NANOTEXNOLOGY 2020, will provide to the participants access to a unique global network of innovators and specialists from the world academic, research and industrial communities.

Front-line experts from multidisciplinary research and application areas joined this conference, to discuss the benefits of N&N in their R&D efforts, to advance the networking and collaborating between different academia, research and industry players in the field and to stimulate the exchange of educational concepts.

NN20 targets the latest developments in the fields of Nanosciences & Nanotechnologies:

- **Plasmonics, Nanoelectronics & Clean Energy**
- **Nanomaterials, Nanofabrication, Nanoengineering & Nanoconstruction**
- **Nanomedicine**
- **Bioelectronics**
- **Graphene and other 2D Related Materials**
- **3D Printing and Bioprinting**

This year we are extremely proud to include in the NANOTEXNOLOGY 2020 and NN20, the

- Workshop on In-line & Real-time Metrology and Quality Control for Nano-Manufacturing,
- Workshop on Computational Modeling of Materials, Devices & Processes, and

On behalf of the NN20 Organizing and International Scientific Committees, we would like to thank you for your participation and support and we ensure that the NN20 presentations, discussions and Round Tables will expand our knowledge and form an outstanding platform for dynamic networking in the N&N fields.

It is our great pleasure to welcome you again to Thessaloniki and we hope that you will enjoy not only the insightful and interesting Scientific Program, but also the exciting networking and social events of NANOTEXNOLOGY 2020!

Best Regards

Professor S. Logothetidis

NN20 Chairman

Contents

NN20 Programme (Greece Local Time Zone)

Monday 6th July

WS3-COVID

11:30-12:00	**KEYNOTE** **Prof. Thomas Webster, Northwestern University, USA** Nanomedicine and COVID-19: Commercializing Improved Prevention, Diagnostic, and Therapeutic Approaches
12:00-12:30	**L. Sideras, Nanotechnology Lab LTFN, Greece** Nanotechnology-based approaches against SARS-CoV-2: Diagnosis and management of COVID-19
12:30-12:45	**K. Tsougeni, Nanoplasmas P.C., Technology Park of NCSR Demokritos (V)** A lab-on-a-chip for rapid, colorimetric detection of SARS-CoV-2 Virus RNA in 30 min post extraction
12:45-13:00	**Heba Nabil Abdelaziz, Arab Academy for science, Technology & Maritime Transport, Egypt** Nano-architecture role in Avoiding viruses impacts in human-built environment

Nanomedicine and COVID-19: Commercializing Improved Prevention, Diagnostic, and Therapeutic Approaches

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As we are in the middle of the COVID-19 pandemic, numerous researchers from across the globe are frantically looking for solutions for improved prevention, detection, and therapies. One area that has received a lot of attention includes the use of materials the same size as COVID-19 itself: nanomaterials. Nanomedicine, or the use of nanomaterials in medicine, provides promise for all aspects of the COVID-19 pandemic as, to just name a few approaches, functionalized nanofibers can provide for improved protection, nanoparticle based biosensors can improve detection sensitivity, and theranostic nanoparticles hold significant promise to both detect and deactivate COVID-19 once in the body. This presentation will cover this as well as other advances nanomedicine is making towards the COVID-19 pandemic, emphasizing those which are currently being commercialized.

Nanotechnology-based approaches against SARS-CoV-2: Diagnosis and management of COVID-19

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Pandemics are not uncommon in themselves and occur again and again at certain intervals. Seen in this way, they are part of evolution.
However, most people are not aware that the death rates are close to those of the world wars. From 1918, the Spanish flu claimed 40-50 million deaths, while the Second World War claimed 50-60 million victims.
Basically, you cannot escape a pandemic; defeat is only possible through the respective immune system. I.e. organizational measures to reduce contact and improve hygiene can only influence the course of the pandemic. Desirable is a method that allows the prognosis of a pandemic with regard to the number of infections as a function of time. This can then be used as a decision-making aid for internal measures and planning / preventive measures in the healthcare system.
For this purpose, a mathematical model of formal kinetics was developed based on the analysis of the biological corona mechanism.
This allowed the experimental, known data on the number of currently actively infected to be modeled as a function of time. Provided that the basic assumptions are valid, the simulation as a whole allows a prediction of the pandemic course.
This is important information for decision-makers when planning measures in all areas.
In addition, nanosilver technology is being worked out as an effective countermeasure in all its facets.

A lab-on-a-chip for rapid, colorimetric detection of SARS-CoV-2 Virus RNA in 30 min post extraction

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Recent viral outbreaks highlight the need for reliable, yet broadly deployable, portable and low-cost diagnostics for the detection of epidemic and emerging infectious agents. We designed, developed and optimized a diagnostic lab-on-a-chip for ultra-fast, visual, colorimetric detection of SARS-CoV-2, the virus that causes the "Coronavirus disease 2020" or **COVID-19.** The lab-on-a-chip is disposable, portable, and cost-effective device. To identify SARS-CoV-2 viral RNA, we used two types of templates: (a) purified synthetic RNA representing the whole viral genome and (b) extracted and purified RNA from nasopharyngeal swabs collected from SARS-CoV-2 positive patients, according to WHO recommended real-time PCR assay. We demonstrate competitive advantages such as high sensitivity (with lower limits of detection of less than 300 copies), ultra-fast analysis (less than 30 min, post RNA extraction), low reagent consumption (25μl), clear color change, and portability requiring only heating and visual inspection. All lyophilized reaction mixtures and reagents are included on the chip in a dry form, allowing room-temperature long term storage for deployment in resource limited settings.

WS3-COVID

Timber Hall 2 & Virtual Room NN (Group A) Chair: C. Gravalidis, Nanotechnology Lab LTFN	
14:00-14:15	**INVITED (L)**
14:15-14:30	**Dr Ilise L Feitshans JD and ScM and DIR** , & Dr Bettina Mues MD MPH Snapshot from the trenches of law and pharmacy: Saving the world from Covid-19 by Applying Nanotechnology
14:30-14:45	**C. Gravalidis, Nanotechnology Lab LTFN, Greece**
14:45-15:00	Predictions on COVID-19 evolution: Status Worldwide
15:00-15:15	**Y. Tang , Western University, Canada (V)** A Mathematical Model of COVID-19 Transmission
15:15-15:30	**Joana C. Antunes, University of Minho, Portugal (V)** Essential oil-loaded chitosan/polyvinyl alcohol blended films and its role as adjuvant to eradicate Staphylococcus aureus and Pseudomonas aeruginosa from infected microenvironments
15:30-15:45	**Richard L Roe, Georgetown University Law Center (V)** Using Nanoenabled Communication to Improve Awareness of Science and Health Education about COVID-19 in Early Childhood Education
15:45-16:00	**Palencia-Aguilar. Carla, GC2M Corp, USA (V)** Nanotechnology Role in the Food Industry to fight against Covid-19

Snapshot from the trenches of law and pharmacy: Saving the world from Covid-19 by Applying Nanotechnology

Dr Ilise L Feitshans JD and ScM and DIR , Dr Bettina Mues MD MPH

Covid-19 requires massive medical relief efforts examined here, from the experience of a pharmaceutical laboratory in Switzerland and from the policy standpoint of operationalizing nanotechnology's revolutionary promises under a cascading rainfall of emergency executive orders and legal predecents from plagues of the past. Promising features of nanotechnology research to cope with the pandemic such as: 3D-Printing: rapid prototyping of highly efficient PPE and other tools against COVID; Cost- effective and rapid point-of-care diagnostics; Nano-biosensors such as the Siddarmark research about and Biomedical Nanotechnology for viruses and bacteria; quick detection and monitoring the traffic and spreading patterns of viral infections; nanofilters against COVID-19;. This presentation offers insights from (1) the history of pandemics, (2) the success story on-site work in the pharmaceutical industry that worked overtime to meet a new and unexpected demand resulted in remarkably low Covid-19 mortality, and (3) emergency executive orders that shape the response to Covid-19. For workers and the families Covid-19 Emergency Executive orders to "stay in place", nanotechnology is a friend offering employment and elearning but increasing their financial hardship when people must absorb overhead without additional support from their employers. This concludes that nanotechnology is vital to Covid-19 response and subsequent economic recovery.

Predictions on COVID-19 evolution: Status Worldwide

C. Gravalidis

Nanotechnology Lan LTFN, Greece

A Mathematical Model of COVID-19 Transmission

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The transmission of disease has been one of the most studied problems by researchers from many disciplines such as epidemiology, applied mathematics, and statistics. Accurate mathematical simulation models for transmission have many meaningful implications in solving challenges of both public and personal health. One such model, the SIR model of disease spread, uses a compartmental approach that includes the dynamic and nonlinear behavior of disease transmission through three factors: number of susceptible, infected, and removed (recovered and deceased) individuals. In this paper, we propose an alternative framework to study the solutions of the SIR model by utilizing the Lambert W function and the Planck Black Body distribution. We then demonstrate the application of the methodology by applying the model to COVID-19 transmission data to model the spread of an infectious disease in a real-world context. Particularly, there will be a brief discussion on the impact of physical distancing practices, and use of personal protection equipment (PPE), on the spread of COVID-19.

Keywords: Lambert W function, Planck Black Body distribution function, SIR model, Nonlinear differential equations, Disease transmission

Essential oil-loaded chitosan/polyvinyl alcohol blended films and its role as adjuvant to eradicate Staphylococcus aureus and Pseudomonas aeruginosa from infected microenvironments

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Chronic wounds (CW) have numerous entry ways for pathogen invasion and prosperity, damaging host tissue and hindering tissue remodelling. Essential oils (EOs) exert quick and efficient antimicrobial (AM) action, unlikely to induce bacterial resistance. Cinnamon leaf oil (CLO) has strong AM properties. Chitosan (CS) is a natural cationic polysaccharide, also endowed with AM features. Its bactericidal activity can be enhanced with CS carrying a lower degree of acetylation (DA), or with quaternary amides turning it permanently cationic (QCS). CS (100-300 kDa; DA of 9.6±1.4%) was further deacetylated in alkaline conditions with/without sodium borohydride to limit depolymerization (DA: 6.8±0.3/5.4±0.2, respectively), and quaternized (QCS) after adding glycidyltrimethylammonium chloride (degree of quaternization of 66%; new FTIR peak at 1475 cm^{-1} representing C-H bending of methyl groups of quaternary amide). Polyvinyl alcohol (PVA; 72 kDa, 88% hydrolyzed) added flexibility and hydrophilicity. CS/PVA films (optimized ratio 30/70; 9%wt) were prepared by solvent casting and phase inversion (similarly as in DOI: 10.1002/app.48626). 0.1% (v/v) CLO was added to CS solution 5 min before blending with PVA, with loading amount based on its minimum inhibitory concentration (19.7 µg/mL for *S. aureus* and 39.3 µg/mL for *P. aeruginosa*, in DOI: 10.3390/antibiotics9060314). Films chemical composition, thermal stability, mechanical properties, permeabilities (air and water) and swelling capability reinforce the achievement of blended films. AM activity (halo test, killing time kinetics, and AM action in dynamic contact at maximum killing time kinetics) increased with CLO and QCS. This study is a first proof of concept that CLO can be dispersed into CS/PVA films and show bactericidal effects, particularly when combined with QCS, opening new perspectives for CW therapeutics.

Using Nanoenabled Communication to Improve Awareness of Science and Health Education about COVID-19 in Early Childhood Education

Richard L Roe, Ketevan Iremashvili Charisma Howell, Ilise L Feitshans

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One key facet of controlling COVID-19 is the need to communicate effectively with the general public in order to implement science-based public health solutions. This is vital for generating essential public support of measures that control transmission and for compliance with preventive measures. One tragic feature of the COVID-19 pandemic is the undermining of the general public's understanding of and belief in the value and quality of sound scientific information for arresting transmission and controlling disease. The public's under-standing of fundamental principles of science/technology and public health (STAPH) must be improved for prevention to be successful. This presentation explains how developmentally appropriate, interactive, learner-centered education in early childhood settings can build a deeper understanding of and appreciation for sci-ence and health among children, their parents and teachers. This is accomplished by hands-on, cognitively and affectively rich learning experiences, and reflection. We will present examples of teaching about COVID-19 utilizing the best practices in experiential education, such as imagination, collaboration, emotional intelli-gence and creativity, to advance effective learning in science, health and nanotechnology. We examine nano-technology that affects children and families (discrimination by inappropriate use of information from nanoenabled biosensors), and demonstrate how nanotechnology can be presented as fascinating to children (3D printing masks) and thereby promote effective learning. We will offer an example of an online curricular model in one area of this learning. Also, we will invite participants to map future directions of educational efforts. In conclusion, quality education can change the course of pandemics through knowledgeable compli-ance with beneficial programs. It behooves civil society to adopt the methods that enable the general public to embrace this destiny.

Nanotechnology Role in the Food Industry to fight against Covid-19

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Nanotechnology in the food industry could be used to fight against Covid-19 in three ways: ***1.*** It can increase the immunological system because the process implemented herein concentrates vitamins, minerals, fiber, proteins, among others. ***2.*** The products can be preserved for periods longer than 2 years without adding any chemicals. ***3.*** The virus within the product will disappear because the molecular sieves are smaller than the virus (10^{-10} versus 10^{-9}), and during the dehydration process, if Covid-19 is present in the unprocessed product, during dehydration, the molecular sieves and biopolymers will allow the virus to attach to their surface, (leaving the product alone), and being destroyed in the regeneration process when the sieves and biopolymers are placed in an oven at temperatures higher than 250°C. The process consists of using clays and biopolymers with sizes from 10^{-6} to 10^{-10} as filters in a vacuum chamber and tuning the changes of temperature and pressure by trial and error until the desired characteristics are obtained. Results showed that: *vitamin content* could increase at least 5 times more than the natural product for the same analyzed quantity, for *inulin content*: 3.5 times more and *probiotics' bacteria count* up to 5 times more. Other advantages include: the system does not use any contaminant substances during the drying process, not abrupt temperature changes take place; therefore, colour and smells are preserved and concentrated; the discharge is only limited to water vapour. More than 1000 products had been tested over a 12 years' research. In addition, subproducts development could result from the recovery of wasted material such as pasta from banana peels, cosmetics from mangostine and shrimp peels, bromelain from pineapple stems, leather from tilapia skins, among others. Whenever subproducts' development is not possible, the waste is used for soil improvement by means of composting.

WS2-Computational

16:30-16:45 16:45-17:00	**KEYNOTE (L)** **M. Damnjanovic, University of Belgrade, Serbia** Topological phases of layers: elementary band representations
17:00-17:15 17:15-17:30	**INVITED (L)** **V. Damljanović, University of Belgrade, Serbia** Electronic Dispersions in Two- and Three-Dimensional Single Crystals FromSymmetry Point of View
17:30-17:45 17:45-18:00	**INVITED (L)** **I. Miloević, University of Belgrade, Serbia** Electronic-band topology of group VI layered transition metal dichalcogenides
18:00-18:15 18:15-18:30	**INVITED (V)** **M. Zacharias, Cyprus University of Technology, Cyprus** Temperature dependence of the optical properties of silicon nanocrystals
18:30-18:45	**E. Antoniou Aristotle University of Thessaloniki, Greece (V)** Ab Initio Computational Investigation of Structure & Magnetic Properties of SmCo5-XNiX Intermetallic Compounds
18:45-19:00	**Ronald Columbié-Leyva, Instituto de Investigación en Materiales, UNAM, México. (V)** Theoretical studies of high-Tc Fe-superconductors based on BaFe2As2 in presence of dopants Rh and Pd.
19:00-19:15	**C. Simserides, National and Kapodistrian University of Athens, Greece (V)** Hole transfer in cumulenic and polyynic carbynes
19:15-19:30	**M. Witkowski , University of Warsaw, Poland (V)** DFT modeling of SERS spectra of dipeptides: A comprehensive study of vibrational structure for Cys-Trp and Trp-Cys adsorbed on Au and Ag

Topological phases of layers: elementary band representations

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Research of topological phases is probably the main stream of condensed matter physics. In brief, Bloch theory transforms band structure of the hamiltonian spectrum into the fibre bundle over Brillouin zone (BZ), in this way enabling topological characterization of such bundles. Extensive work is performed within differential-geometric framework: Berry phase and derived notions (connection, curvature and Wilson loop e.g.), are used to find topological invariants like winding and Chern numbers. However, 30 years ago Mischel and Zak, pathed the symmetry based combinatorial way to classify band structures. Reconsidered recently, these results are firmly related to topological phases of crystals. This purely algebraic method considers graphs graphs imposed by symmetry. The first one is graph of Brillouin zone: as a contractible manifold, each stratum of ***k***-vectors with equivalent (conjugated) stabilizers is a vertex of the graph, while (oriented) edges connect neighbouring strata. Bands are made of patches over strata, each corresponding to specific allowed irreducible representation (IR) associated to the stratum. Contraction of BZ to graph, causes simultaneous contraction of the band patches, and the whole band structure becomes IR-graph: vertices are IRs, while edges represent connected patches. These edges are subdued to compatibility relations, or better, they depict them. Therefore, having BZ-graph, and compatibility relations (the both are directly and fully symmetry-determined), all possible IR-graphs are found in a combinatorial manner. This procedure is implemented in POLSym code, and applied to all layer groups (single and double, with or without time reversal). The results are presented, together with various analyses. For example, the disconnected graphs are looked for, as pointing out topologically non-trivial phases. Also, selected are band structures with special subgraphs which indicate possible atomic limits.

Electronic Dispersions in Two- and Three-Dimensional Single Crystals From Symmetry Point of View

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In spatially periodic atomic arrangements, the electronic energy depends on the wave vector and forms a band structure. The form of a band in the vicinity of some point in the Brillouin zone is called the electronic dispersion and determines many physical properties of a material. Examples of electronic dispersions are Dirac (e.g. in graphene), semi-Dirac (e.g. in black phosphorus) and quadratic (e.g. in MoS_2). On the other hand, every crystal periodic in two (three) directions belongs to one of 80 layer- (230 space-) groups. Here we present deep connection between the crystal symmetry and the types of electronic dispersions present in the crystal. Our contribution is based on works published for two- [1-3] and three-dimensional [4-7] single crystals. We show that new and unexpected types of dispersions often appear as a consequence of crystal symmetry. This may be the clue for discovery of new materials with interesting physical properties.

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Electronic-band topology of group VI layered transition metal dichalcogenides

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Group VI layered transition metal dichalcogenides (TMDCs) exist in multitude forms. Such a variety of configurations manifests itself in diverseness of their electronic properties making them extremely interesting as potential key-elements of sophisticated functional devices.
Here we analyse electronic-band topology of the broad spectrum of TMDC structures: from 2H, 1T and 1T' monolayer phases to plethora of stacking patterns of TMDC few-layered structures.
To this end, we use program POLSym in which we have incorporated subroutines based on topological quantum chemistry establishing symmetry relations between localized and extended crystal states in two-dimensional materials. The POLSym code outputs complete set of irreducible representations and elementary band representations of Layer Groups (LGs) together with Double-LGs, Gray-LGs and Double-Gray-LGs, thus enabling full-symmetry-based study of electronic-band topology of layered compounds with spin degree of freedom, time reversal symmetry and spin-orbit interaction.

Temperature dependence of the optical properties of silicon nanocrystals

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Silicon nanocrystals (SiNCs) have been under active investigation in the last decades and have been considered as a promising candidate for many optoelectronic applications [1]. Some of the fundamental properties of interest in these nanostructures is the temperature dependence of their optical absorption onset, and how this is controlled by different passivation regimes [2]. In this talk we present first-principles calculations performed in conjunction with the special displacement method [3] to study the temperature dependence of the band gap renormalization of free-standing hydrogen terminated, and oxidized SiNCs, as well as matrixembedded SiNCs in amorphous silica. Our results exhibit good agreement with experimental photoluminescence data [2]. We also provide strong evidence that the electron-phonon interplay at the surface of the nanocrystal is suppressed by oxidation and the surrounding amorphous matrix. For the matrix-embedded SiNCs, we show a high correlation between the temperature dependence of the band gap and the Si-Si strained bonds [4]. This result emphasizes the immanent relationship between electron-phonon coupling and thermal structural distrotions. We also demonstrate that, apart from quantum confinement, Si-Si strained bonds is the major cause of zero-phonon quasidirect transitions in matrix-embedded SiNCs.

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Hole transfer in cumulenic and polyynic carbynes

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We study hole transfer in open cumulenic (equidistant carbons) and polyynic (alternating long-short distances between carbons) carbynes [1-4], atomic nanowires made of *N* carbon atoms, using Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) and utilize few Tight-Binding (TB) Wire Model variants: a simplistic wire model with all sites equivalent and models with modified end sites, mimicking the existence of 1 or 2 or 3 hydrogens at the edge sites. For RT-TDDFT we mainly use B3LYP and basis sets 3-21G, 6-31G*, cc-pVDZ, cc-pVTZ, cc-pVQZ, obtaining clear convergence. With DFT, RT-TDDFT and TB variants we study energy spectra, density of states, ground state energy, the formation of energy gap between occupied and empty eigenenergies, charge as well as electric dipole moment oscillations, mean over time probabilities to find the carrier at each site, coherent transfer rates and frequency content. We consider cumulenic molecules with coplanar (co) or perpendicular (pe) methylene end groups as well as polyynic molecules starting with short (sl) or with long (ls) C-C bonds and ending in CH- or CH_3- end groups, for odd or even *N*.

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Ab Initio Computational Investigation of Structure & Magnetic Properties of $SmCo_{5-X}Ni_X$ Intermetallic Compounds

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Modern technological applications in an extensive variety of fields require the use of Permanent Magnets (PMs). Limited availability and high cost of the necessary raw materials in manufacturing of PMs have increased the need to develop innovative materials. Intermetallic compounds such as $SmCo_5$ are already used as high-performance PMs. Reducing the high content of the expensive cobalt in $SmCo_5$ from low-priced transition metals can lead in a cost reduction. Specifically, this study examines by computational methods the effect of substituting cobalt atoms in the hexagonal crystal structure of $SmCo_5$ by nickel atoms. The aim is to specify the structure that will be stable and at the same time will maintain high values of magnetization.
VASP is used to perform the atomistic simulations. The calculations are based on Density Functional Theory. Various simulations are performed by considering all the possible crystallographic positions on Co and Ni atoms in $SmCo_{5-x}Ni_x$ intermetallic compound. The cases are evaluated on the basis of energy minimization and maximizing the magnetization.

Acknowledgement: “This research is co-financed by Greece and the European Union (European Social Fund- ESF) through the Operational Programme «Human Resources Development, Education and Lifelong Learning 2014-2020» in the context of the project “Ab initio computational investigation and experimental growth & characterization of advanced materials for permanent magnets.” (MIS 5047849).”

DFT modeling of SERS spectra of dipeptides: A comprehensive study of vibrational structure for Cys-Trp and Trp-Cys adsorbed on Au and Ag

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Surface-enhanced Raman scattering (SERS) phenomenon, emerging from adsorption of molecules onto plasmonic surfaces and resulting in increase of the intensity of Raman scattering signal by a few orders of magnitude, is becoming widely employed in the studies of various molecules, including peptides. Adsorption of short peptides can be achieved efficiently *via* thiol group of cysteine (Cys), which can bind to surface of silver and gold; while tryptophan (Trp), exhibiting considerable Raman cross-section due to its aromaticity, increases overall signal-to-noise ratio of measured spectra. All these features make Cys-Trp and Trp-Cys ideal candidates for model molecules in studying SERS effect. Although SERS spectra of such molecules are dominated by vibrations of Trp moiety, small changes in the overall structure can have a significant impact on the spectrum. In our recent work (A. Królikowska *et al*., *J. Phys. Chem. C* 2020, 124, 13, 7097–7116) we discussed this problem in detail, exploring systematically the SERS response of dipeptides with important alterations, such as the order of amino acids, covalent modification of terminal group(s) and particular type of plasmonic surface used. This presentation is focused on the computational aspect of that work, where using density functional theory (DFT) methods we were able to calculate the optimised geometry and theoretical vibrational spectra of systems composed of dipeptide and metal cluster (with a few silver or gold atoms). Potential energy distribution (PED) analysis facilitated the full interpretation of all experimental SERS spectra, allowing for thorough understanding of the vibrational structure of the system. Combining theory and experiment showed that SERS response of studied dipeptides is strongly influenced by the main-chain direction and type of terminal modification, when various substrate types and/or excitation wavelengths are compared.

Theoretical studies of high-T_c Fe-superconductors based on $BaFe_2As_2$ in presence of dopants Rh and Pd.

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The superconductivity has a long history. One of the recent discoveries is the superconductivity in the Fe- based family with anti-ferromagnetic state at ambient temperature. The pure material $BaFe_2As_2$ is a semi-metal and has not superconductivity. The transition to the superconductivity state appeared in presence of different dopants. In this report we present the results of calculations using the embedded cluster method [1,2] at the RO-MP2 electron correlation level and two suites of programs MOLPRO 2020 and Gaussian 16. The cluster $Ba_4Fe_5As_8$ in presence of Rh and Pd as dopants was used. The NBO population analysis showed two main features: the independence of charge density transfer from the spin density transfer and, the presence of orbitals with electron density but without spin density. The observed properties correspond to the RVB mechanism for the superconductivity proposed by Anderson for cuprates. This confirmed the conclusions made in our publications for the same material doped by Co and Ni [3,4].

References:

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2. I.G. Kaplan, J. Hernandez-Cobos, J. Soullard, Quantum Systems in Chemistry and Physics, 143–158 Kluwer Academic, Dordrecht (2000).
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5.

Tuesday 7th July

WS1

11:00-11:30	**WELCOME** **Prof. S. Logothetidis, NN20 Chairman**
11:30-12:00	**KEYNOTE (V)** **R. Silva, University of Surrey, UK** Powering the next generation of Wearables and IoT with Plastic Electronics
12:00-12:30	**INVITED (V)** **J. Briscoe, Queen Mary University of London, UK** Scalable fabrication and treatment of hybrid perovskite solar cells by aerosol-assisted chemical vapour deposition
12:30-12:45	**Ieng-Wai. Un, Ben-Gurion University of the Negev, Israel (V)** Thermal effect in plasmon assisted photocatalyst: a parametric study
12:45-13:00	**Ieng-Wai. Un, Ben-Gurion University of the Negev, Israel (V)** Thermo-Optical Nonlinearity of Metallic Nanoparticle(s)

Powering the next generation of Wearables and IoT with Plastic Electronics

S. Ravi P. Silva
Advanced Technology Institute, Department of Electrical and Electronic Engineering, University of Surrey, Guildford, Surrey GU2 7XH, United Kingdom.

The world is advancing at an unprecedented rate due to modern electronics led by communication technologies around us. Is this the 4th Industrial Revolution, which is more a convergence of technologies around us to single platforms with multi-user and multi-functionality, to serve both for manufacture and social integration? It is predicted that there are over 50 billion IoT devices at present facilitating the accurate mapping and information gathering, allowing for modern lifestyles with high quality of life. Each second another 127 devices are connected to the internet, with the IoT market exceeding US$1 trillion by 2023.

What powers the IoT, with the ability for these devices to become wireless and autonomous? At present the favoured energy source is Li-ion batteries but this is not sustainable. With the increasing wireless sensors and high complexity of wearables it is not difficult to see the need for millions of tons of scarce lithium; which is not realistic. An alternate route to powering the IoT is via advances in energy scavenging led by the plastic electronic revolution taking place. In this talk I will describe how flexible solar and flexible triboelectric nanogenerators (TENGs) are creating a mini-revolutions themselves with the advances being made on efficiency, power delivery and sustainability. The future of the IoT will be tied to the available wireless power that will be dependent on modern energy scavenging technologies. The plastic electronic community will be able to facilitate these needs due to the advantages it has in form-factors, low-weight, energy capability and technologies available. The proposed energy solutions will also contribute to e-skins and virtual energy sources for modern integrated building materials in large area electronics. ***Ref:*** J. Zhang et al. Materials Today (2020); W. Li et al. J. Mater Chem C (2020); RDIG Dharmasena et al. Proc. IEEE (2020) & Nano Energy (2020).

Scalable fabrication and treatment of hybrid perovskite solar cells by aerosol-assisted chemical vapour deposition

J. Briscoe
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Aerosol assisted chemical vapour deposition (AACVD) is a scalable deposition process, and a key advantage of this method compared to conventional CVD is the fact that the precursors do not need to be vaporized. This allows for lower operating temperature, less complex equipment, and therefore lower overall cost. We previously demonstrated the first ever deposition of continuous methyl ammonium lead iodide (MAPI) films using this method. However, films were of the order of 1-5 µm thick, and therefore not suitable for photovoltaic (PV) devices. I will discuss how we have developed this process to form thinner films down to 500 nm, with large, monolithic grains of 2-10 µm in diameter. These films were then used to fabricate working photovoltaic devices in the n-i-p structure: a first for films made via AACVD.

Furthermore, we recently have developed this method to use as a post-deposition treatment on existing films, modulating the morphology and boosting the performance of conventionally spin-coated MAPI films to over 20% PCE. We show through a combination of structural (including high-res STEM-HAADF), electronic and optical techniques that this enhanced efficiency is achieved through a combination of reduced grain boundaries and 'healing' of the perovskite structure with a more intrinsic, lower defect character with longer charge-carrier lifetimes. We have also demonstrated that this technique can be used on a range of compositions, device architectures and deposition methods, as well as large-area, HTL-free and thick (<1 µm) devices, providing efficiency enhancements in all cases. This post-treatment approach also proves to enable highly-controlled tuning of the film morphology, including the formation of ultra-large grains. Through this we have studied the variation in optoelectronic properties across such grains at the nanoscale, which will also be discussed.

Thermal effect in plasmon assisted photocatalyst: a parametric study

Ieng-Wai. Un[1], Yonatan Sivan[1],

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Recently, it has been suggested that chemical reactions can be facilitated by using mm-scale composites of metal nanoparticles on porous metal oxides when illuminated at their plasmonic resonance wavelength. This effect was shown recently to be predominantly associated with the heating induced by illumination [Y. Sivan, I.W. Un & Y. Dubi, Chem. Sci., 2020]. In this work, we study the parametric dependence of the temperature distribution in these composites numerically, and provide analytic expressions for simple cases. It turns out that the physical picture emerging from the collective thermal response is quite different from the one emerged from the single particles. We show that since these systems are usually designed to absorb all the incoming illumination, the temperature rise distribution in them is typically is weakly-dependent on the illumination wavelength, pulse duration, particle shape, size and density. In contrast, we also show that the temperature rise distribution is strongly sensitive to the beam size and the thermal conductivity of the host oxide [Y. Sivan& I.W. Un, submitted]. These results have a direct implication in the route for optimization of the reaction rates. This study is an important step towards a better understanding of thermal effects in conventional photocatalytic experiments. On the more general level, this work would also be instrumental in uprooting some common misconceptions associated with the role of thermal effects in plasmon-assisted photocatalysis and other applications that rely on heat generation from a large number of particles.

Thermo-Optical Nonlinearity of Metallic Nanoparticle(s)

Ieng-Wai. Un[1], Yonatan Sivan[1],

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The thermal effect is known to be one of the strongest mechanism of optical nonlinearity but is usually avoided under ultrafast illumination. In this work, quite different from many previous studies in the ultrafast region, we study the thermo-optical nonlinearity of a single metal nanoparticle and many-nanoparticle composite under continuous-wave illumination. We show that the thermo-optical nonlinearity of single metal nanoparticle system is strongly dependent on the illumination wavelength and the nanoparticle size. The results of the single nanoparticle system are then used to study the thermo-optical nonlinearity of many-nanoparticle composites. We show that, different from the case of a single nanoparticle, the thermo-optical nonlinearity of the composite is strongly sensitive to the thermal conductivity of the host material only. These results are critical for the optimization of the photo-thermal effect in many applications. More importantly, since photo-thermal effects were shown to be responsible for observations of faster chemical reactions, our results can be used to interpret correctly the differences in chemical reaction enhancements originating from the thermo-optical nonlinearity at different illumination intensities.

WS1	
14:00-14:15	**INVITED (V)**
14:15-14:30	**O. L. Muskens, University of Southampton, Highfield, Southampton, UK** Tunable and smart metal oxide infrared metasurfaces for radiative cooling of satellites and multiband flat optics
14:30-14:45	**E. Papis-Polakowska , Łukasiewicz Research Network-Institute of Electron Technology, Poland (V)** Passivation of InAs/GaSb type-II superlattice photodetectors using long-chain thiol self-assembled monolayers
14:45-15:00	**V. A. Klinkov Peter the Great St.Petersburg Polytechnic University, Russia (V)** Development of thermoplastic glass for the formation of microlenses on the semiconductor surface
15:00-15:15	**INVITED (V)**
15:15-15:30	**Aris Christou, University of Maryland, USA** Material and Nanostructure Challenges for Wide Bandgap Switches with THICK Homo and Hetero -GaN Epitaxy
15:30-15:45	**KEYNOTE (V)**
15:45-16:00	**Prof. Theodore Moustakas, Boston University, USA** Development of UV LEDs for environmental and medical applications

Tunable and smart metal oxide infrared metasurfaces for radiative cooling of satellites and multiband flat optics

O. L. Muskens[1], K. Sun[1,2], I. Zeimpekis[3], W. Xiao[1], M. Simeoni[4], A. Urbani[4], M. Gaspari[4], S. Mengali[4], M. Zalkovskij[5], L. Kildebro[5], N. Kalfagiannis[6], D. W. Hewak[3], C. H. de Groot[2]

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Efficient temperature control of spacecraft during missions requires high performance and durable radiative cooling panels. New thin-film solutions can offer cost and weight advantages compared to existing technology. Recently we have developed a new approach based on an infrared metasurface perfect absorber with very low solar absorption, exploiting the plasmonic effects in doped metal-oxides such as Al:ZnO (AZO) [1]. AZO with tunable carrier densities was fabricated using atomic layer deposition by varying the Al-doping and deposition temperature. As an alternative to using conventional physical patterning by etching or liftoff, we present a new strategy using an oxygen plasma to control the carrier density in AZO [2]. A patterned SiN hard mask is used to locally block the effects of the plasma, resulting in modulation of carrier density on length scales below 100 nm. The plasma oxidation process is used to achieve planar metasurfaces without any surface topography. The complete absence of texturing is of interest for complex multilayer designs and, for example, we have demonstrated a multiband metasurface by integrating a visible-range metasurface on top of the planar infared AZO metasurface with low mutual cross-talk. Our current research proceeds towards achieving smart radiation control using a temperature dependent emissivity metasurface including VO_2 as a thermochromic material, aimed at maintaining a stable window of operation for spacecraft in a changing environment [3].

[1] K. Sun et al., ACS Photonics 5, 495–501 (2018)
[2] K. Sun et al., Adv. Mater. (2020), DOI: 10.1002/adma.202001534.
[3] K. Sun et al., ACS Photonics 5, 2280–2286 (2018)

Passivation of InAs/GaSb type-II superlattice photodetectors using long-chain thiol self-assembled monolayers

E. Papis-Polakowska[1], K. Czuba[1], T. Runka[2], T. Martynski[2] A. Jasik[1]

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Type-II InAs/GaSb superlattice (T2SL) has received increasing attention as the alternative material to HgCdTe alloy for the next generation of infrared photodetectors and focal plane arrays due to improved stability, reduced Auger recombination and unwanted tunneling currents. Unfortunately, GaSb-based devices suffer from the surface oxidation being one of the surface-leakage currents sources. Furthermore, the appearance of an elemental Sb gives rise to the conduction path parallel to the interface. Passivation is the most effective method to eliminate these problems and improve the performance of devices. Chemical deposition of the thiol self-assembled-monolayers (SAMs) is a novel approach to the passivation of T2SL detectors. In this work, we present a complementary study of (100) GaSb and (100) InAs surfaces covered with alkane and aromatic thiols. Generally, the SAMs spontaneously deposited on a semiconductor surface can be used both for passivation of surface and bio- and chemical sensing. In our work, the surface chemistry was analyzed using Raman spectroscopy and surface morphology was examined by atomic force microscopy. The contact angle measurements have been used for the characterization of the surface properties on the macroscopic scale. The passivation efficiency has been determined by current-voltage characteristics measurement. The two-step passivation with the octadecanethiol-based wet treatment followed by SiO_2 deposition allowed for a reduction of the dark current by one order of magnitude for T2SL detectors. Furthermore, the results showed one of the most important aims of the passivation, namely long term stabilization of the passivated surface. In addition, the thiol SAMs are promising in the context of their use in the virus and bacteria sensors - necessary and important systems in the current special time.

Development of thermoplastic glass for the formation of microlenses on the semiconductor surface

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The infrared region 1-10 μm are of great practical importance for gas control, medicine, biosensorics and laser systems. Advances in the development of compact high-performance semiconductor and solid-state radiation sources in the indicated spectral region allow to obtain new classes of sensor devices on their basis. Existing optical materials cannot be used as passive elements in the mid-IR range due to the limited transmission region. In addition, they cannot be used in fused deposition modeling (FDM) and 3D printing techniques. The paper presents the results of a physical and chemical study on the development of a thermoplastic glassy material for optical microlenses for semiconductor LEDs and photodiodes. An optical cell based on such optocoupler operating in the spectral range of 3.4 μm and 4.3 μm is the basis of compact methane and carbon dioxide sensors, respectively. The following requirements were imposed on the glassy material: low optical losses, high refractive index (to reduce the critical angle of the emitted radiation), softening temperature above 200˚C, which provide the use of glass melt extrusion system and microlens formation on optocoupler in a single technological process. As a glassy system satisfying the above requirements, chalcogenide glasses based on As-S-Se-(I) compositions were selected. The study developed an automated system for applying microlenses to semiconductor heterostructures, and established the influence of the shape and height of the lens on the external quantum yield of LEDs. The conducted experimental studies allowed us to increase the minimum sensitivity and signal-to-noise ratio of gas sensors based on a semiconductor optocoupler by 2-5 times. This research work was supported by the Academic Excellence Project 5-100 proposed by Peter the Great SPbPU “Development of glassy and composite materials for biosensors and smart medicine devices”.

Material and Nanostructure Challenges for Wide Bandgap Switches with THICK Homo and Hetero -GaN Epitaxy

Aris Christou

Materials Science Department, University of Maryland, College Park, Maryland, USA

The current state of GaN bulk crystal growth technology and GaN epitaxy lags behind the state of many of the compound semiconductor technologies especially in meeting the power device requirements for thick epitaxial layers beyond 10 microns thickness. ***This presentation reports the results of the UMD investigations on the characterization of defects in thick GaN epitaxial layers, doped and undoped leading to an understanding of the parameters which influence defect propagation*** from the substrate into the epilayer, as well as the results of our investigation of the electrical activity of defects in thick (10s–100s of μm) epilayers. ***Our focus has been to investigate the morthology and the spatial statistical distribution of defects through experimental defect characterization investigations as well as to develop the appropriate probability density functions for spatial distribution as well as thickess distributions.***

Thick GaN and related nitride epitaxy is required for achieving high speed power switching beyond 2 kV. We have applied advanced defect spectroscopic techniques to thick epi materials and two-terminal test structures. These include: deep level transient spectroscopy (DLTS), photoconductivity spectroscopy, photo-induced current transient spectroscopy (PICTS), and photoluminescence (PL) spectroscopy. epilayer, as well as the results of our investigation of the electrical activity of defects in thick (10s–100s of μm) epilayers ***as well as the spatial distribution and thickess distributions.***

Development of AlGaN UV LEDs for environmental and medical applications

Theodore D. Moustakas

Department of Electrical and Computer Engineering, Boston University, Photonics Center, Boston MA 02215, USA

High efficiency ultraviolet (UV) light sources are in grade demand for a number of environmental, medical and industrial applications. Such include, for example, water and air sterilization, disinfection of surfaces, phototherapy, free-space non-line-of-sight communications, UV curing and printing, counterfeit detection, and fluorescence identification of biological/chemical agents. Currently mercury lamps are used for the majority of these applications. The UN Minamata Convention on Mercury took effect on August 2017, and mandates the progressive elimination of use of mercury. UV LEDs based AlGaN alloys, whose energy gap varies with composition from 3.4 eV (365nm) to 6.2 eV (200nm), covers the entire UV spectral region and thus, can be used as an alternative to mercury lamps. This talk addresses the materials and devices issues, which need to be resolved, in order to form efficient UV LEDs based on AlGaN alloys. Due to the lack of native substrates AlGaN UV-LEDs are generally grown heteroepitaxially primarily on (0001) sapphire substrates, and have a high concentration of dislocations. Furthermore, oxygen incorporation due to the high chemical affinity of Al for oxygen leads to high concentration of non-radiative recombination centers in high Al-content AlGaN alloys. Both the high dislocation density and the incorporation of oxygen impurities limit the internal quantum efficiency (IQE) of the AlGaN-based UV-LED. I will describe a new method of growth, which leads to AlGaN alloys free of oxygen impurities and band structure potential fluctuations. Injected electron-hole pairs in such devices are localized in these band structure potential fluctuations, which leads to efficient radiative recombination. Device architecture issues to increase the carrier injection efficiency (IE) in the active region of the device and light extraction efficiency (EE) from such UV LED devices will be addressed.

WS2-Thin-Films

Timber Hall 2 & Virtual Room NN (Group A)	
16:30-16:45	**KEYNOTE (V)** **Fabrizio Pinto, Izmir University of Economics, Republic of Turkey**
16:45-17:00	Dispersion force engineering and next-generation spacecraft: Case studies in a nanoscale emerging enabling general-purpose technology
17:00-17:15	**K.Emmert, Fraunhofer ISC, Germany (V)** Biodegradable functional coatings for sustainable packaging solutions: bioORMOCER®
17:15-17:30	**A. C. Papageorgiou Technical University of Munich, Germany (L)** Emerging Complexity in Two-Dimensional Molecular Architectonics with Linear Bis-Hydroxamic Acid Modules on Surfaces
17:30-17:45	**Sunghwan Lee Purdue University, United States (V)** Thermodynamic-based synthetic strategies of p-type oxides for thin film transistor applications
17:45-18:00	**P. Knotek University of Pardubice, CZ (V)** Photo-induced Solid State Reaction at the Interface of the Multilayer GeSe – AsS System
18:00-18:15	**S.Yu. Turishchev, Voronezh State University, Russia (V)** On the possibility of microspot advanced studies of the E.coli bacteria surface
18:15-18:30	**Alexe C.A. INCDTP- Division Leather and Footwear Research Institute, Romania (V)** Multifunctional Leather Surfaces Covered With Nanocomposites Through Conventional And Unconventional Methods

Dispersion force engineering and next-generation spacecraft: Case studies in a nanoscale emerging enabling general-purpose technology

Fabrizio Pinto[1]

Department of Aerospace Engineering, Faculty of Engineering, Izmir University of Economics, Teleferik Mahallesi, Sakarya Cd. No:156, 35330 Balçova/İzmir, Republic of Turkey

Speculation regarding mechanisms to allow binding among the basic constituents of matter can be considered to have originated even as the concept of atom was introduced in the 5th-4th centuries BC, from philosophical arguments, by Leucippus and Democritus in the Thracian city of Abdera, to the east of Thessaloniki. This occurred because the problem of change could not be addressed by only hypothesizing atoms without a means to connect them to one another. Despite such purely philosophical beginnings, the existence of interactions between boundaries was often recognized from direct workshop experience culminating, at the end of the 19th century, with the invention of the Johansson blocks. Possibly, this was the first technology entirely enabled by engineering forces between surfaces interacting across sub-micrometer distances, several decades before London's quantum mechanical theory of dispersion forces. After recalling the key principles, we shall review notable examples of modern industry products enabled by these interactions, such as the atomic force microscope (AFM), and novel non-volatile memory elements (NEMS). Even as our understanding was growing that dispersion force engineering can lead to breakthrough technological applications on the nanoscale, the spacecraft industry was evolving along a trajectory decisively prizing smaller payload mass thus taking advantage of vastly reduced launcher costs. The manner in which dispersion force engineering as an emerging general purpose technology can enable spacecraft miniaturization is the core focus of this Keynote Talk.

Biodegradable functional coatings for sustainable packaging solutions: bioORMOCER®

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Biodegradable films for packaging represent a promising way to contribute to a more sustainable society. However, state-of-the-art bio-based packaging films often do not meet all the necessary requirements. These bio-based packaging films usually have insufficient barrier properties and cannot guarantee the required shelf life for food. Therefore, bio-based films have only had limited use as high-quality packaging materials up to now. For this reason, Fraunhofer ISC developed biodegradable functional coatings, which equip the bio-based films with the desired properties.

Our so called ORMOCER® (inorganic-organic hybrid polymers) exhibit excellent barrier properties towards gases and vapors and thus can be used as functional coatings in food packaging materials. However, the state-of-the-art ORMOCER® is not biodegradable. To realize new biodegradable ORMOCER® based coatings, several suitable biodegradable precursors have been identified (e.g. chitosan, cellulose derivatives, polycaprolactone-triol (PCL-T)). The new material class bioORMOCER® was obtained by nano-chemical incorporation and chemical linkage of the chemically modified bio-precursors into the ORMOCER® matrix.

BioORMOCER® coatings are biodegradable, transparent and provide very good barriers. The coatings show good adhesion on various surfaces and can also be used as planarization layer. The kinetics of biodegradability is temporally adaptable. This variety of adjustable properties opens a wide field of further possible applications. For example, tests of different ORMOCER® systems for biomedical purposes are underway.

Emerging Complexity in Two-Dimensional Molecular Architectonics with Linear Bis-Hydroxamic Acid Modules on Surfaces

A. C. Papageorgiou[1], C. Jing[1], B. Zhang[1], S. Synkule[1], M. Ebrahimi[1], A. Riss[1], W. Auwärter[1], L. Jiang[1], G. Médard[2], J. Reichert[1], J. V. Barth[1]

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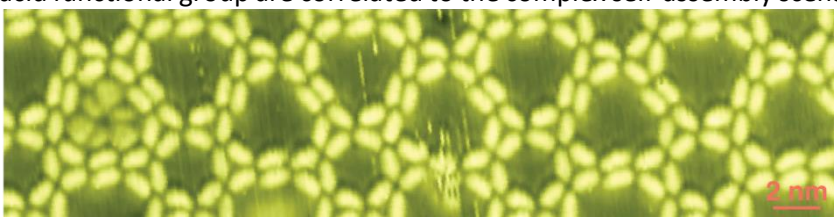
Recently, we functionalised linear building blocks with two terminal hydroxamic acid groups and applied them to two-dimensional (2D) architectonics on the close-packed single crystal surfaces of silver and gold [*Angew. Chem., Int. Ed.* 58 (2020) 18948]. A combination of scanning tunnelling microscopy, atomic force microscopy, X-ray photoelectron spectroscopy and density functional theory investigations found that the molecular building block would ever so slightly adapt its shape in the environment provided by the supporting surface and its neighbouring molecules. This affords an unusual manifold of surface supramolecular motifs: two to six molecules held together by intermolecular interactions. Only a handful of these motifs organised in 2D crystals, ranging from close-packed structures to polyporous networks. Dynamic, chiral supramolecules formed enantioselectively within some of the larger network pores, demonstrating chirality transfer from host to guest (see figure). Molecular coverage, as well as the chemical state of the hydroxamic acid functional group are correlated to the complex self-assembly scenario.

STM micrograph of polyporous network on a silver surface.
Each rod corresponds to a single molecule. Fuzzy features indicate mobile species. A ‚clockwise propeller' guest supramolecule is discerned.



Thermodynamic-based synthetic strategies of p-type oxides for thin film transistor applications

Sunghwan Lee[1], Huachao Mao[1], and Xingyu Wang[1]

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Oxide electronics have gained prominence in recent years and have been established as one of the most promising new-technologies for next generation displays. The high potential-use seen in oxide electronics is due primarily to their high carrier mobilities and their ability to be fabricated at low-temperatures. However, the vast majority of oxide semiconductors are n-type oxides, which limits the current applications to unipolar devices and ultimately stunts the development of oxide-based complementary metal-oxide-semiconductor (i.e., CMOS) devices. In this presentation, we report on a thermodynamic-based in-situ synthesis of nonstoichiometric p-type oxides of which the formation reaction depends on the oxide/metallization interfacial reaction stability and instability. Thin films of oxides and metals were deposited using ultra-high vacuum magnetron sputtering at room temperature and low-temperature interfacial reaction annealing was made to synthesize p-type oxides. Further, we integrated the successfully synthesized p-type oxides into thin film transistor (TFT) test devices. The fabricated TFT devices demonstrate descent device performance with clear drain current saturation behaviour, on/off current ratio greater than 10^3, the max field effect mobility of ~ >4 cm^2/Vs. The defect-based doping mechanism and carrier transport behaviour governed by ionized-impurity scattering will also be discussed. The thermodynamic-based synthetic strategies of p-type oxides presented here may resolve the scientific questions that limit the realization of p-type oxides and their electronic and optoelectronic device applications.

Photo-induced Solid State Reaction at the Interface of the Multilayer GeSe – AsS System

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Department of General and Inorganic Chemistry, University of Pardubice, CZ
Joint Laboratory of Solid State Chemistry, University of Pardubice, CZ

This study is focused on the photo-induced changes in double-layered thin As-S and Ge-Se films evaporated on each other. Due to the similar values of refractive indexes of single layers the photo- and thermo- induced changes from UV-Vis spectra according to the Tauc´s model were analyzed. The changes of the Tauc band-gap energy (ΔE_g^{opt}) of the double-layer film $(As_2S_3)_x(Ge_{30}Se_{70})_{1-x}$ were significantly higher in the comparison to the sum of the changes of individual layers induced by the identical conditions. These significantly higher values of ΔE_g^{opt} are attributed to the fact, that during exposure a solid state reaction occurred on the interface region (layer). Driving force for this reaction was the thermodynamic more advantageous formation of the Ge-S bonds in this system. The FTIR, optical ellipsometry, AFM and DSC analysis confirmed the presence of newly formed Ge-S and As-Se bonds, which were induced by the illumination or annealing under an inert atmosphere. The role of radiation´s wavelength on the photoinduced changes (ΔE_g^{opt}) and its influence on reaction´s kinetic were studied in the next step. The 532 nm laser illumination provided the highest (ΔE_g^{opt} ~ 115 meV) and quickest (reaction rate constant k = 12.1 min^{-1}) changes due to the suitable penetration depth and energy of the photons. The annealing at the temperature 172 °C led to the similar changes of the ΔE_g^{opt} ~ 106 meV. The role of the evaporation order, chemical composition and thickness of individual layers were also studied. Laser induced threshold of illumination was determined at exposure by the high-intensity 532 nm source.

On the possibility of microspot advanced studies of the E.coli bacteria surface

S.Yu. Turishchev[1], D. Marchenko[2], V. Sivakov[3], E.A. Belikov[1], O.A. Chuvenkova[1], E.V. Parinova[1], D.A. Koyuda[1], R.G. Chumakov[4], A.M. Lebedev[4], T.V. Kulikova[1], A.A. Berezhnoi[1], I.V. Valiakhmedova[1], E.V. Preobrazhenskaya[5] and S.S. Antipov[1,5,6]
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The combination of a few nanometers inorganic particles with nature-like objects can play a crucial role in engineering of novel low-dimensional hybrid materials. One of the convenient objects for such kind of technology development is E.coli bacterial culture. The surface properties play an important role for such systems. PhotoEmission Electron Microscopy (PEEM) can play a key-role by providing the powerful ability to perform chemically sensitive small spot spectromicroscopy surface analysis at one time. The crucial point is bio-objects stability under special conditions of surface sensitive vacuum experiments.

X-ray photoelectron spectroscopy (XPS) and Scanning Electron Microscopy (SEM) control studies were performed before and after PEEM experiments with E.coli cells. PEEM images were collected under Hg lamp irradiation and with the use of tunable high intensive synchrotron light. Obtained results demonstrate a possibility of effective PEEM bioimaging of the E.coli cells under "hard" conditions. The surface topology of single bacteria has been detected by PEEM that well correlates with the SEM studies results. Only partial bacteria shell damage have been shown. Our observation strongly suggests that PEEM spectromicroscopy surface analysis can be applied up to a single E.coli cell structure and composition studies without significant bioobject destruction.

The study was supported by Russian Science Foundation (Project 19-72-20180). Russian-German Lab provided PEEM Microscope facility supported by BMBF grant No.05K12KE1.

Multifunctional Leather Surfaces Covered With Nanocomposites Through Conventional And Unconventional Methods

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In this paper we present the results obtained by depositing the nanocomposite materials based on nano TiO_2/TiO_2:N, Ag, SiO_2, carbon nanotube, single-walled, carboxylic acid functionalized (SWCNT-COOH), poly(2,2' bithiophene)- PBTh and poly(dipheylamine)- PDPA by conventional and unconventional methods on the surface of sheepskin leathers. The nanocomposite materials were integrated in film forming polymers and were applied on sheepskin leather surfaces by spraying (conventional method) or by activating the surface with cold atmospheric plasma followed by electrospraying (unconventional method). The leather surfaces were tested for antimicrobial properties against Gram-positive and Gram-negative bacteria and fungi according to ISO 20743: 2007. The photocatalytic properties under visible light exposure were also tested using two organic stain models (methylene blue and orange II). The stain discoloring was evaluated by measuring the color differences between the blank and the samples with DATA Color Check Plus II portable device assisted by CIELab color management software. The evaluation of the physical-mechanical resistance and comfort properties for the sheepskin leathers was determined by measuring the water vapor permeability, rubbing tests and abrasion resistance. The results showed that the sheepskin leather surfaces treated with nanocomposite materials have improved antibacterial, self-cleaning, physical-mechanical and comfort properties as compared to untreated samples, with potential applications for added value multifunctional products.

Acknowledgements: This work was funded by Romanian Ministry of Education and Research, CCCDI - UEFISCDI, within PNCDI III, in the frame of projects no. 44/2018_ PHYSforTeL and no. 6PFE_4PERFORM-TEX-PEL/2018.

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PLENARY	
19:00-19:30	Introduction by Prof. S. Logothetidis, ISFOE20 & NN20 Chairman
19:30-20:15	**Controlling hybrid inorganic/organic electronic materials interfaces** N. Koch[1,2,3] [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany [3]Institute of Functional Nano & Soft Materials, Soochow University, China
20:15-21:00	**Matter-to-Life: How to Build a Cell** J.P. Spatz Max Planck Institute for Medical Research, Heidelberg, Germany

Controlling hybrid inorganic/organic electronic materials interfaces

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Electronic and opto-electronic devices rely on a precise control of the charge density distribution, which is the key parameter for electronic and optical processes in devices. The charge density and its energy spectrum in electronic materials determine elemental parameters and functions, such as the Fermi level position, type and mobility of charge carriers, interfacial energy level alignment, carrier injection and extraction at contacts, and the characteristics of excitations. The primary conventional method to control the charge density in electronic materials is doping. However, established electronic materials and doping concepts, e.g., the statistical incorporation of dopant atoms in a covalent lattice, will soon reach fundamental limits. The anticipated route beyond this deadlock is the use of new electronic materials and combinations thereof, where tuning quantum confinement and the charge density enable new device concepts. In this contribution, at first the fundamental differences in the electronic properties of selected advanced and emerging electronic materials are contrasted, i.e., organic semiconductors, metal halide perovskites, and two-dimensional transition metal dichalcogenide monolayers. Next, considerations of how the energy levels differ in practical thin films from those in single crystals will provide the basis for discussing fundamental interfacial phenomena in hybrid heterostructures comprising dissimilar material classes. Modern approaches to tune the interfacial charge density re-arrangement, and concomitantly the energy level alignment, will then be introduced and their impact on interface functionality in devices exemplified. Most of these approaches are based on employing very strong molecular electron donor or acceptor molecules as interlayers, and photochromic molecular switches even facilitate *operando* optical control over electrical device characteristics, i.e., multifunctionality.

Matter-to-Life: How to Build a Cell

J.P. Spatz

Max Planck Institute for Medical Research, Heidelberg, Germany

The evolution of cellular compartments for spatially and temporally controlled assembly of biological processes was an essential step in developing life by evolution. Synthetic approaches to cellular-like compartments are still lacking well-controlled functionalities, as would be needed for more complex synthetic cells. With the ultimate aim to construct life-like materials such as a living cell, matter-to-life strives to reconstitute cellular phenomena *in vitro* – disentangled from the complex environment of a cell. In recent years, working towards this ambitious goal gave new insights into the mechanisms governing life. With the fast-growing library of functional modules assembled for synthetic cells, their classification and integration become increasingly important. We will discuss strategies to reverse-engineer and recombine functional parts for synthetic eukaryotes, mimicking the characteristics of nature's own prototype. Particularly, we will focus on large outer compartments, complex endomembrane systems with organelles and versatile cytoskeletons as hallmarks of eukaryotic life. Moreover, we identify microfluidics and DNA nanotechnology as two highly promising technologies which can achieve the integration of these functional modules into sophisticated multifunctional synthetic cells.

Wednesday 8th July

WS3

11:00-11:30	**INVITED** **Prof. Yannis Missirlis, University of Patras, Greece** Information and communication pathways in cells
11:30-11:45 11:45-12:00	**INVITED (V)** **Dr. Gerard Tobias, Institut de Ciència de Materials de Barcelona, Spain** Biomedical imaging and therapy with carbon nanotubes
12:00-12:15	**A. Mavromanoli, Aristotle University of Thessaloniki, Greece** The use of electrospraying for the production of polylactic-co-glycolic acid-based propolis nanoparticles
12:15-12:30	**M.Bartolewska , University of Warsaw, Poland (V)** Preparation of gold nanoparticles with sulforaphane as a reducing agent.
12:30-12:45	**N. C. Homem, University of Minho, Portugal(V)** Functionalization of CA/PCL wet-spun microfibers with essential oils for biomedical applications
12:45-13:00	**K. Polak, University of Warsaw, Poland (V)** Potential Active Pharmaceutical Ingredients - metacetamol and its new crystalline forms

Information and communication pathways in cells

Yannis F.Missirlis

Multicellular organisms maintain life, genesis, growth and development, homeostasis until death, by receiving and transmitting a multitude of signals effecting their behaviour.
Signals may have an external origin, or be generated inside the organism, may be physical or biochemical, may be focused or diffused.
There are signals which travel at different speeds, at various distances, using special transduction pathways; They can be stopped before reaching their target, or attenuated, or even «hijacked». Most organisms are entities where an interplay between somatic and bacterial cells and viruses share the same space. Their information and communication pathways may cross each other, accidents may happen leading to specific pathologies.
It may be , therefore, that the information technology communication systems have their counterpart in the biological world. This means that security aspects such as passwords, encryption techniques, hacking and other disturbances are used also by the cells for their physiological processes.
A reverse biomimetics approach should be explored in an attempt to understand better signal transduction in living organisms.

Biomedical imaging and therapy with carbon nanotubes

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Carbon nanotubes have been advocated as promising agents for in vivo imaging, tumour targeting and drug delivery systems. When carbon nanotubes are combined with inorganic compounds, the resulting hybrid materials benefit not only from the properties of their constituent nanomaterials but also from synergistic effects.

The most explored approach consists on the external decoration of carbon nanotubes with inorganic nanoparticles. One advantage of using carbon nanotubes though is that their inner cavity can be employed for the encapsulation of a chosen payload. The outer surface remains available and can be subsequently modified to attach biomolecules with the aim of improving the dispersability and biocompatibility of the developed hybrids. Even for targeting agents can be anchored to the external surface.

In this talk we will see some examples on both the external decoration of carbon nanotubes with inorganic nanoparticles and the encapsulation of a variety of inorganic payloads. The resulting hybrid materials find application in biomedical imaging and as therapeutic agents.

The use of electrospraying for the production of polylactic-co-glycolic acid-based propolis nanoparticles

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Introduction: Propolis is a multipotent substance manifesting a great deal of beneficial properties against oxidation, inflammation, neoplastic growth and immunity disorders. Its oral administration results in rapid degradation mostly in the gastrointestinal tract. The encapsulation of propolis in polylactic-co-glycolic acid (PLGA)-based nanoparticulate systems would be very promising for controlled propolis release with low toxicity, improving its physicochemical properties and bioavailability.
Materials-Methods: Electrospraying with the application of particulate voltage has been used for the production of propolis nanoparticles, carried by the polymeric compound PLGA. Organic solvents have been suitable both for propolis and PLGA working solutions. Cytotoxicity studies have been carried out for the evaluation of the safety of the nanoparticles produced.
Results: PLGA has been successfully used for the polymeric encapsulation of propolis in nanoparticulate systems. Coherent and stable nanoparticles with a narrow size-distribution around 40nm have been produced with the electrospraying technique. Methylene blue and MTT studies have indicated the safety of these nanoparticles.
Discussion: PLGA-based propolis nanoparticles produced by electrospraying could be used for large-scale production of controlled drug delivery systems in several medical applications. Further research has to be done in this direction with the ultimate goal to incorporate such nanosystems in everyday life.

Preparation of gold nanoparticles with sulforaphane as a reducing agent.

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Gold nanoparticles (AuNPs) is an important class of nanomaterials applicable in biomedical domain. AuNPs have been widely employed for diagnostic and therapeutic purposes. On the other hand, among various potent anticancer agents, D,L-sulforaphane (SF) has been shown to be very effective against many different types of tumors.

In this work, we report on the synthesis of gold nanoparticles (Au-NPs) through reduction of gold precursor with sulforaphane. The size and morphology of the Au-NPs was controlled by changing the composition of the reaction mixture and the temperature. It is demonstrated that sulforaphane reacts with $AuClO_4^-$ ions and its decomposition products are likely adsorbed onto the surface of the forming nanoparticles which governs their further growth.

The resulting structures have been examined with a range of physicochemical methods including dynamic light scattering, electron microscopy, and spectroscopic techniques. Depending on the reaction conditions spherical or flower-like structures have been obtained. The synthesized particles appear to be a new promising material for medical applications like drug delivery or diagnostics.

Functionalization of CA/PCL wet-spun microfibers with essential oils for biomedical applications

N. C. Homem[1], J. C. Antunes[2], M. A. Teixeira[3], A. R. M. Ribeiro[4], M. T. P. Amorim[5], H. P. Felgueiras[6]
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Essential oils (EOs), which are complex biomolecules composed of volatile compounds, have emerged as a new strategy to deal with bacterial infections and as a valid alternative to synthetic drugs in the treatment of chronic wounds (CW) by promoting the regeneration of damaged tissues. Here, we report the modification of biodegradable wet spun microfibers composed of cellulose acetate (CA) and polycaprolactone (PCL) with EOs, aiming at their controlled release. Cinnamon leaf oil (CLO), cajeput oil (CJO), and clove oil (CO) were selected according their minimal inhibitory concentration (MIC) against *Staphylococcus aureus* (< 22.4 µg/mL) and *Escherichia coli* (< 11.2 µg/mL). CA/PCL prepared at 10% and 14% wt in 3:1 ratio in acetic acid and acetone was processed in the form of microfibers in a lab scale wet-spinning set-up, being extruded at 0.5 mL/h directly into an ethanol coagulation bath at RT. Microfibers were modified by immersion for 72 h under low stirring (RT, 200 rpm) in ethanol solutions containing EOs at 2xMIC and ampicillin (control antibiotic). Incorporation was confirmed by UV-VIS, FTIR and TGA. After 72h, fibers contained ampicillin at MIC (control), but only 14% MIC of CLO, 66% MIC of CO and 76% MIC of CJO. Microfibers were observed by brightfield microcopy and characterized as uniform and homogeneous even after EO immobilization. Data showed that even at small amounts the EO-modified microfibers were more effective than the ampicillin-modified fibers against the tested bacteria. Most importantly, CLO-containing fibers were the most effective from the group, suggesting the active groups within their composition have a superior affinity towards the CA/PCL fibers, therefore increasing their antimicrobial potential even at smaller amounts. These results indicate that CA/PCL microfibers loaded with EOs can be easily produced and applied in scaffolds for the treatment of CW.

Potential Active Pharmaceutical Ingredients - metacetamol and its new crystalline forms.

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Before launching a new drug to the market, one has to provide a complete description of all possible polymorphic forms of the compound as required by regulations of the Federal Food and Drug Administration (FDA). Presented information on those polymorphs is very important since any changes in the crystal structure can result in differing physical properties of an API such as stability, dissolution rate, and others.

Paracetamol (N-acetyl-para-aminophenol) is an example of a widely used pain relief drug with three known forms of polymorphs indicating different physical properties. Since it has been proved to be hepatotoxic, searching for its substitutes became very important in the pharmaceutical industry. One of the candidates for this application is metacetamol (N-acetyl-meta-aminophenol) – structural isomer of paracetamol. This compound gained a lot of attention due to the research providing the evidence of its less hepatotoxicity.

Until now, in the Cambridge Structural Database (CSD) we can find several records regarding the structures containing metacetamol. In this research, we present two new metacetamol solvates. Their crystal structures have been investigated in detail along with a comparison with pure metacetamol and its hydrated form.

I3D

11:00-11:30	**INVITED** **Evangelos Delivopoulos University of Reading, RG66AY, UK** An alginate fibre scaffold as a spinal cord organoid
11:30-11:45	**INVITED** **Prof. Ioanna Zergioti, National Technical University of Athens, Greece** Laser Induced Forward Transfer as a tool for precise bioprinting
11:45-12:00	
12:00-12:15	**Carlos Carvalho, EnvisionTEC GMBH, Germany** 3D Bioplotter Over 15 Years of Bioprinting
12:15-12:30	**A. Shannon University of Limerick** Radiopaque 3D printing for medical application
12:30-12:45	**INVITED**
12:45-13:00	**Prof. Aylin Sendemir, Ege University, Turkey** Utilisation of Microfluidics in 3D Bioprinting

An alginate fibre scaffold as a spinal cord organoid

Dr. Evangelos Delivopoulos[1]
School of Biological Sciences, University of Reading, RG66AY, UK

The emergence of hydrogels during the past decade has stimulated a rapid growth in tissue engineering. Scaffolds from different materials consist of three dimensional environments that encapsulate pluripotent stem cells in a specified geometry. These scaffolds have adjustable mechanical properties and enable the targeted delivery of chemical compounds, such as morphogens and drugs, to the encapsulated cells. Alginate is a naturally derived, biocompatible hydrogel, commonly used for 3D cell culture. Previous experiments have used alginate hydrogels to differentiate encapsulated embryonic stem cells (ESCs) to a range of cell fates *in vitro*. Here we demonstrate a fibre scaffold based on alginate of two different molecular weights (low and high). We used SEM imaging to investigate the porosity of hydrogels from the two alginates and monitor encapsulated cell adhesion to the scaffold. Cell viability remained above 50% for both low and high molecular weight alginates. With 3D printing we can engineer a gradient of growth factors that can direct embryonic stem cell fate into a neuronal lineage and propose a 3D alginate platform for the patterned neuralization of embryonic stem cells, using retinoic acid and smoothened agonist, which are both promoters of neural phenotypes. Immunofluorescent staining and gene expression analysis via PCR reveals the presence of differentiated neuronal precursors within the alginate scaffolds. Our method can be used to investigate the influence of localised cell signalling gradients, while our platform is a valuable model of the developing neural tube and can reveal regeneration strategies for spinal cord injury. We envision a time when spinal cord organoids will be ready as transplants for paraplegic and quadriplegic patients.

Laser Induced Forward Transfer as a tool for precise printing of biomolecules and drug products

Ioanna Zergioti
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Laser Induced Forward Transfer (LIFT) process has been utilized as a novel microfabrication tool for the printing of a plurality of organic and inorganic materials, both in liquid and in solid phase, with dimensions down to a few microns. LIFT is a direct-write method that can print viable bioinks including living cells in predefined 2D or 3D patterns. It is contact-less process which offers high spatial control (10-100μm) and is able to print a great variety of materials in terms of viscosity. Our group has recently developed an innovative approach based on this technique, capable of the direct printing of biomolecules and their immobilization in a single step, thereby significantly reducing the time and cost required for the creation of biopatterns. The approach involves the formation of functional hydrogel networks onto receiving surfaces with biomolecules incorporated into them in a spatially controlled and contactless manner. In particular, the direct printing and immobilization of enzymes, antibodies and cells has already been demonstrated by the NTUA group, on suitably substrates for biosensing and regenerative medicine applications.
The use of different 3D printing technologies for pharmaceutical manufacturing provides new opportunities for personalized medicine and on-demand tailored drug products, such as implants and other dosage forms. In this work we present our recent achievements in developing a viable manufacturing process for printed personalized dosage forms onto thin films. The main advantage of LIFT printing lies in the preparation of thin films as dosage forms, each with different designs, multiple actives and sizes. The obtained thin films were characterized regarding their recovery, disintegration time and homogeneity.

3D Bioplotter Over 15 Years of Bioprinting

Dipl. Chem. Carlos Carvalho, Process & Material Development, EnvisionTEC
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Abstract: Three dimensional (3D) bio printing is the utilization of 3D printing–like techniques to combine cells, growth factors, and biomaterials to fabricate biomedical parts that maximally imitate natural tissue characteristics. Generally, 3D bio printing utilizes the layer-by-layer method to deposit materials known as bio-inks to create tissue-like structures that are later used in medical and tissue engineering fields. Bio printing covers a broad range of biomaterials.

Radiopaque 3D printing for medical application

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Majority of 3D printing technologies use polymers as their base material. However, polymers are ordinarily radioloucent, meaning they do not show up clearly under x-ray imaging. Polymer-based medical devices would therefore be invisible under medical imaging such as standard x-ray imaging, CT/microCT imaging and fluoroscopy. A radiopaque 3D printing resin would increase opportunities for 3D printing as a method to manufacture medical devices (or components part of) and implants to be visible when x-ray imaged. This material could also be used to create anatomical phantoms and calibration aids for medical imaging. As part of this research, a 3D printable radiopaque resin was developed and successfully 3D printed. This consisted of a commercially available biocompatible resin impregnated with zirconium oxide nanoparticles. Viscosity and UV curability of the resin were not compromised with the addition of the nanoparticles. This study demonstrates a method to create radiopaque artefacts using Polyjet 3D printing technology, but could be adapted to other printing methods. A model of a hand printed with and without the radiopaque ink are shown below.

Utilisation of Microfluidics in 3D Bioprinting

Prof. Aylin Sendemir

Ege University, Turkey

"Bioprinting" is defined as the development of tissue constructs using a set of techniques that deposit biocompatible materials and cells (bioinks) onto a substrate with computer-aided, specialized 3D printers to construct 3D functional living structures. Extrusion type bioprinters combine the advantages of multiple cell/material delivery, higher viscosity and direct incorporation of cells and bioactive molecules. However, in order to print large and intricate structures, material properties have to be optimized. "Printability" of bioink is an intricate issue, where cell viability and resolution drops as the viscosity and shape fidelity is increased. Besides, there is considerable amount of shear stress during printing, which further decreases the cell viability.

Integration of microfluidic systems into bioprinting equipment provides considerable advantages in:

- improving cell viability by reducing applied shear stress,
- precise manipulation of volume of bioinks to be extruded, therefore improving resolution, control of morphology, dimensions and direction,
- simultaneous extrusion of multiple inks through the same nozzle, thus allowing to fabricate heterogeneous structures that better mimic the native ECM and cellular organization,
- creation of complex patterns, graded or layered structures.

After further optimisation of processing techniques and standardisation, the use of microfluidic-based 3D bioprinting is expected to enable the development of a broad range of functional tissues with complex structures for many important applications.

WS2-Nanoparticles

14:00-14:15	**INVITED (V)**
14:15-14:30	**M. R. Koblischka Saarland University, Germany** The possible applications of superconducting nanowire network fabrics
14:30-14:45	**EU PROJECT (L)** **Ch. Panagiotopoulou National Technical University of Athens (NTUA), Greece** Study of the influence of the addition of closed- structure expanded perlite microspheres on the density and compressive strength of cement pastes
14:45-15:00	**EU PROJECT (V)** **F. Antolini ENEA Photonics Micro and Nanostructures Laboratory, Italy** High performance quantum dots synthesis, photo-lithography/direct laser patterning and micro-LED/OLED sources for RGB micro-display manufacturing: the MILEDI project
15:00-15:15	**Mahmoud Omar, Université Laval, Québec, Canada. (V)** Synthesis and radiolabelling of ultrasmall colloidal nanoparticles for skin permeation measurements using a novel method based on nuclear imaging (PET)
15:15-15:30	**Palencia-Aguilar.Carla, GC2M Corp USA (V)** Nanotechnology in Water and Oil Applications
15:30-15:45	**S. Stan, VDL Enabling Technologies Group, The Netherlands** SCIL – An Emerging, Advanced Nanoimprinting Technology

The possible applications of superconducting nanowire network fabrics

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In this contribution, we discuss the possible applications of superconducting nanowire network fabrics or fiber mats. Such materials can be prepared using the electrospinning technique or the blow-solution technique, using sol-gel derived precursor materials. In a first step, a network of polymer nanowires is obtained containing the ceramic precursor materials. In a second step, the heat treatment, the ceramic reaction takes place and the samples are oxygenated to form the superconducting phase. The resulting samples consist of polycrystalline nanowires with nanometer-sized grains, and the nanowires are interconnected on multiple places with each other, which enable the flow of supercurrents through the entire perimeter of the sample. The nanowire network fabrics exhibit an extremely low weight due to the small density of ~0.05 g/cm^3, but the samples were found to carry superconducting currents even in applied fields of up to 10 T, despite their polycrystalline nature. This makes the nanowire fabrics suitable for all applications where the weight of the superconducting material counts. One advantage of both fabrication techniques is the scalability which enables the growth of large-scale superconducting samples, which is currently not possible with other preparation techniques. The resulting fullyreacted fiber mats are very brittle, but shaping of the samples is possible in the green stage. The selected shape is conserved in the necessary oxygen treatment to obtain the superconducting phase. This enables the preparation of very specific sample shapes, e.g., for magnetic shielding. Another possibility is the fabrication of foils using a low-temperature withstanding polymer. Several more types of applications are outlined as well.

Study of the influence of the addition of closed- structure expanded perlite microspheres on the density and compressive strength of cement pastes

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The current trend in the construction industry is the development of ever lighter-weight elements and components that can at the same time maintain the good mechanical properties of traditional construction materials. The addition of lightweight aggregates, including expanded perlite, in concrete is one of the most common techniques used for density reduction of cementitious products. Nevertheless, one of the main drawbacks attributed to conventional expanded perlite, which affects the final product properties, is the increased water absorption that this material exhibits due to its high porosity.

Expanded perlite microspheres (EPMs) is a novel, low cost material that uniquely combine important properties rendering it an ideal filler; it is tiny, spherical, inert, lightweight, thermal insulating, with closed external surface and considerable mechanical properties. We produced 4 EPM grades of different density (67 to 233 kg·m^3) by implementing indirect heating technology in Vertical Electric Furnace (VEF) and we incorporated them in cement pastes. The addition level (0.0-0.4 ml perlite/g cement) of each perlite quality in cement pastes with w/c ratio of 0.35 was investigated through the analysis and evaluation of the density and compressive strength of the final cementitious products. SEM/EDS measurements were performed on selected samples, in order to evaluate the microstructure of the developed products, which is known to affect their mechanical properties.

The conclusions of the present study will include the effect of i) the expansion degree ii) quantity iii) the morphological and structural properties (such as grain shape, porosity and compressive strength) of the expanded perlite, on the development of the density, compressive strength and morphology of the final cementitious products.

High performance quantum dots synthesis, photo-lithography/direct laser patterning and micro-LED/OLED sources for RGB micro-display manufacturing: the MILEDI project

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In this work, some of the advances on the European project MILEDI (www.miledi-h2020.eu) are reported and commented.
The MILEDI goal is to demonstrate that QDs can be used as photo-emissive material for color down conversion of a blue micro-LED/OLED source to realise a RBG micro-display. The patterning technologies explored within the project to obtain the pixels are the direct laser patterning and the photolithography. The direct laser patterning method is explored to obtain in a single step the QDs starting from a specified precursor. On the other side the photolithography is used as tool to pattern QDs at high resolution for the realisation of a RGB micro-display. Some examples of the direct laser patterning are reported to show how the laser pulses can generate cadmium based QDs. A particular emphasis is given to the cadmium-free QDs synthesis showing the QDs high optical performances that are implemented in the photolithographic patterning. Micro-LED and OLED sources manufacturing is another key step to exploit the potential of the QDs and patterning technologies explored within the MILEDI project.
The micro-display is designed to be integrated in a rear projector for car interior or for augmented reality applications. In the second year of the project, the chemistry of the QDs synthesis, the implementation of the direct laser patterning and photolithography and the micro-LED/OLED source manufacturing is illustrated.

Synthesis and radiolabelling of ultrasmall colloidal nanoparticles for skin permeation measurements using a novel method based on nuclear imaging (PET)

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Diffusion cells are used in the pharmacological sciences to measure the permeation of molecules (and nanoparticles) across biological and polymeric membranes (e.g. skin, polymer gloves). Unfortunately, in the case of certain highly potent compounds such as nanoparticles carrying anti-cancer drugs (i.e. “nanocarriers”), the detection technologies currently used in diffusion cells (UV-vis, FTIR) are not sensitive enough. A diffusion cell operating in a positron emission tomography scanner (PET) was designed (Figure 1.a-b) as a new tool to improve the sensitivity in diffusion studies and to allow real-time monitoring. We report on radioactive nano-colloids (ultrasmall $^{89}Zr_{(IV)}$-gold nanoparticles–GNP), as a model nanocarrier for testing with PET, the permeation of nanoparticles (and large molecules) across membranes. GNPs (4nm diam.-TEM; hydrodynamic diam. 19nm diam.-DLS) were grafted with deferoxamine, DFO (chelator for $Zr_{(IV)}$; Figure.1.c), and their physicochemical properties were characterized by FTIR, XPS, TGA, and elemental analysis. Radiolabeling was performed with $^{89}Zr_{(IV)}$ (half-life: 3.3days; 95% radiochemical yield; Au:Zr molar ratio: 1:1.7). FTIR revealed the presence of DFO at the surface of GNPs (hydroxamate peeks: 1629.0cm^{-1}, 1569.0cm^{-1}; amine peek: 3312.0cm^{-1}). XPS revealed the O=C–N C1s peek of DFO at 287.49eV. and upon $Zr_{(IV)}$ chelation, chelated $Zr3d_{5/2}$ peek at 182.4eV with no ionic $Zr3d_{5/2}$ (183.38eV). The permeation of GNPs through skin was studied with PET (Figure.1.d-f). ^{89}Zr-GNPs were detected at a concentration as low as 6.8x10^{-06}nM of ^{89}Zr-DFO and 2.2nM of Au. Real-time monitoring revealed Au penetrated in the skin and out with influx 7.8 µM mm^{-2}hr^{-1} and 4.9 µM mm^{-2} hr^{-1}, respectively. This study confirms the strong potential of PET

as a high-sensitivity, real-time imaging instrument to monitor the permeation process of biomedical nanoparticles across biological membranes.

Nanotechnology in Water and Oil Applications

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Vacuum Clay-Nanofilters with molecular size of 3Å open new possibilities on water treatment. The technology can be used either to destroy undesirable cells, transform or recover desirable ones. For the first scenario, experimental results showed that from seawater in Cartagena-Colombia port, with initial number of cells count of 8 cells/g at 1:1 dilution; after the Clay Nano-filter process, at 1:100 dilutions, less than 100 cells/g were found; and seawater with sediments at 1:100 dilutions with 12000 cells/g before the treatment, after the process, at the same dilution, there were less than 100 cells/g. For the transformation and recovery scenario: three oil based components with different viscosities were tested with seawater mixes of 50%-50% and 25% of oil and 75% of seawater with changes in pressure and temperature, in a 12-hour cycle and 24-hour cycle. The former showed water removal results between 65% to 80%. The latter from 69% to 81%. The Clay-Nanofilters allowed the separation oil-seawater without adding more substances facilitating the possibility of oil reuse for the same application and for lower grade mineral products. Treated engine oil under the Vacuum Clay- Nanofilters technology contained higher values (in ppm) in elements such as Mo, B, Mg, P and Zn than not treated engine oil, but they were within the acceptable ranges for reusable oils. Other results reinforced the fact that Vacuum Clay-Nano filters technology reduces elements' content of Al, Cu, Fe, Na, Si and Ca and destroys Cr, Pb, Sn and K within the reusable product. The undesirable elements that left the system in a gas form were recaptured by biopolymers for pollution control.

SCIL – An Emerging, Advanced Nanoimprinting Technology

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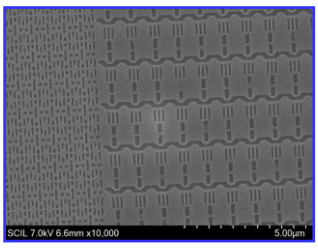
The nanoimprinting technologies are steadily paving the way in the manufacturing of many electronic components. Many applications like augmented reality, healthcare and microbiology, energy harvesting, optical communications, anti-counterfeiting, etc. require nanostructures that enable devices to perform at the cutting edge of their performance and can be manufactured at low cost as well. Examples of such devices are micro LEDs, bio-MEMS, integrated photonics, laser arrays and advanced solar cells. Substrate Conformal Imprint Lithography (SCIL) solves the limitations of the nanoimprinting lithography (NIL) processes by enabling excellent resolutions, avoiding pattern deformations, allowing precise overlay and prolonging the reusability of the stamp. Three series of SCIL equipment are available for processing wafer-type substrates at R&D/pilot scale (LabSCIL), in volume production (AutoSCIL 200) and fab-integrated high volume (FabSCIL 200/300).



I3D

14:00-14:15	**INVITED**
14:15-14:30	**A. Tasolamprou Foundation for Research & Technology-Hellas (FORTH), Greece** Fabrication and characterization of Fused Deposition Modeling 3D printed mm-scaled metasurface units for microwave applications
14:30-14:45	**Panagiotis M. Angelopoulos, National Technical University of Athens, Greece** ABS/ expanded perlite microspheres filament for 3D printing of lightweight and thermal insulating components through Fused Filament Fabrication method
14:45-15:00	**M. Maturi, University of Bologna, Italy** Phosphorescent Bio-Based Resin for Digital Light Processing (DLP) 3D-Printing
15:00-15:15	**C. Theocharatos, Computer Vision Systems, IRIDA Labs S.A., Greece** An embedded vision-based solution for closing the loop in Additive Manufacturing
15:15-15:30	**A. Orfanos, BL Nanobiomed P.C., Greece,** Novel fabrication of 3D printed non disposal face masks
15:30-15:45	**JAC Sy, Industrial Technology Development Institute, Philippines** Effect of gamma irradiation on the mechanical and physicochemical properties of Stereolithography (SLA) 3D printed Formlabs Grey resin
15:45-16:00	**E.S. Vasilyeva, Peter the Great St. Petersburg Polytechnic University, Russian Federation** Development of a machine for the manufacture of micro-optical lens and layered geometric forms of chalcogenide

Fabrication and characterization of Fused Deposition Modeling 3D printed mm-scaled metasurface units for microwave applications

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We present a cost-effective, eco-friendly and accessible method for fabricating three-dimensional, ultralight and flexible millimeter-scale metasurfaces using a household 3D printer. In particular, we fabricate conductive Spilt Ring Resonators, SRRs, in a free-standing form, employing the so-called Fused Deposition Modeling 3D printing technique. We experimentally characterize the samples through transmission measurements in standard rectangular waveguide configurations. The structures exhibit well defined resonant features dependent on the geometrical parameters and the infiltrating dielectric materials. The 3D printed components are suitable for practical real-life applications while the method holds the additional advantage of the ecological approach, the low cost, the flexibility and the small weight of the components. Thus, the flexible and light metasurfaces may serve as electromagnetic components and fabrics for coating a plethora of devices and infrastructure units of different shapes and size.

ABS/ expanded perlite microspheres filament for 3D printing of lightweight and thermal insulating components through Fused Filament Fabrication method

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3D printing constitutes a revolutionary technology that experiences continuously expanding applicability to numerous industrial sections. However, the predefined physicochemical and thermal properties of existing thermoplastic filaments set strong limitations to the application of 3D printing manufacturing method for the production of functional components with specific properties for demanding applications.

We have developed a new type of composite filament that consists of Acrylonitrile butadiene styrene (ABS) as binder and expanded perlite microspheres (EPM) as filler. EPM are tiny cellular particles of low density, closed external surface and high sphericity, and they are produced through the innovative technology of indirect heating in a Vertical Electric Furnace (VEF). EPMs possess low bulk density (< 250 $kg \cdot m^{-3}$) and thermal conductivity (< 0.05 $W \cdot m^{-1} \cdot K^{-1}$). We produced different types of EPM and incorporate them into the ABS aiming to synthesize different composite filament grades, in terms of the EPM size and filler/binder ratio, using a melt extruder under optimized conditions. The filaments were used for the preparation of dog-bone samples in a classical 3D printer of modified nozzle through Fused Filament Fabrication method.

Composite filaments and dog-bone samples were characterised in terms of their density, thermal conductivity, mechanical properties and morphology. It was shown that the new type of composite filaments can be easilty manufactured on a conventional melt extruder, and the composite filament can be used for the production of lightweight and thermal insulating elements of satisfactory strength using conventional 3D printing technology for the first time in the literature. EPMs' properties affect both filament formation and 3D printing, while particles of low diameter and higher density possess optimum performance in both processes.

Phosphorescent Bio-Based Resin for Digital Light Processing (DLP) 3D-Printing

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Since the advent of polymer-based 3D printing technologies, the scientific community has directed great efforts towards the development of new polymeric formulations that would allow to apply this technique to the most various fields of application, ranging from material science to tissue engineering. However, most of the available materials are nevertheless oil-based and cost-effective. This work present a novel bio-based resin for stereolithographic DLP 3D Printing formulated by mixing a photocurable polyester obtained from renewable resources (poly(1,3-propanediyl-co-glyceryl) itaconate-co-vanillate, PPGIV) with methacrylated citrate and itaconate crosslinkers (bis(HEMA) itaconate, BHI and tris(HEMA) citrate, THC) and appropriate photopolymerization initiators, terminators and dyes. As a proof-of-concept, the photocurable ink is formulated with minimal amounts of phosphorescent Ir(III) cyclometalated complexes and its potential applications has been demonstrated for both rigid and flexible structures.

An embedded vision-based solution for closing the loop in Additive Manufacturing

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A vision-based solution for closing the loop in Additive Manufacturing (AM) is presented, providing an effective process control for interrupting the 3D printing procedure in case of critical process failure. The goal is to monitor the AM process with a comprehensive vision sensing system that interacts with the machine process algorithms in order to detect and correct deposition errors, therefore compromising the shape of the manufactured part or the material properties and contributing towards zero-defect AM procedure. To accomplish that, the vision sensing system is comprised of different optical sensors, monitoring three different aspects of the AM process/product, namely the 3D geometry, the temperature profile of the part under production, as well as the melt pool of the laser deposition process. A stereo vision system is used to accurately create a 3D model of the part under production. Sensorial data are processed by a software tool that constructs a 3D point cloud, which can be then compared to the nominal CAD files of the parts to define geometrical differences that are made during the AM process. The interoperable vision system assesses the surface quality and product's properties, enhanced by an IR camera that performs thermal profiling and characterization. In addition, a comprehensive vision system for process control consisting of an optical camera integrated on the scanner head for monitoring size, shape and temperature of the melting pool is included. The solution performs on-camera image processing directly on the camera's FPGA for closed-loop AM melting process monitoring. Live monitoring of the melt pool geometry on the working surface during the deposition allows to optimize the overall procedure, by tuning, in real-time, the process parameters (like laser power, laser head velocity, feed rate and powder mass stream) in a closed-loop configuration process.

Novel fabrication of 3D printed non disposal face masks

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The COVID-19 pandemic is profoundly challenging health systems, national economies and the governance structures of global health. COVID-19 has infected more than 7 million people and is already the deadliest pandemic with over 400.000 deaths the last 6 months. Public mask wearing is most effective at stopping the spread of the virus. However, most of the commercially available masks do not achieve the level of contaminant reduction provided by a certified respirator, as they cannot seal properly the face. Thus, there is currently a high demand of proper designed masks. 3D printing is a very cost-effective way to massively produce this kind of equipment.
In this work, we designed and 3D printed a face mask capable of adjusting properly on the face. Each part of the model was designed and printed separately in order to achieve a design of the highest quality. We used CAD Programs (Fusion360 and Blender) to design each part. After slicing the model's files and determining the printing parameters, we proceeded to the final step, i.e. applying the Fused Deposition Modeling (FDM) technique. We used different polymer materials, in filament form, to 3D print the various parts of the masks. We strongly believe that the current model of 3D printed non disposal face mask, in combination with proper nanofilters, offers the highest possible protection against contamination of the virus.

Effect of gamma irradiation on the mechanical and physicochemical properties of Stereolithography (SLA) 3D printed Formlabs Grey resin

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A standard sterilization method for most medical devices is gamma irradiation. Gamma sterilization offers several advantages because it allows sterilization of samples at room temperature without heating and avoids risk of possible re-contamination because the irradiation can be performed directly in the material's definitive packaging. This work investigates the effect of the gamma irradiation on the tensile, physical and chemical properties of the Stereolithography (SLA) printed polymer. SLA printed specimen and parts were 3D printed using commercial Formlabs Grey resin, then were exposed to gamma-ray doses of 50 kGy. The suitability of gamma rays for sterilizing SLA printed medical parts was evaluated considering the specimens' mechanical and physicochemical properties. The tensile strength 3D printed specimens were obtained following the ASTM D638 method using the Instron 5585H Model UTM at a conditioned atmosphere of 23±2 ^{o}C and 50±5% relative humidity. The irradiation actually increased the tensile strength of the material. The FTIR spectra of both the unirradiated (control) and irradiated samples were obtained using Perkin Elmer FTIR Spectrometer Frontier using the Attenuated Total Reflectance (ATR) Technique at a scan range of 4000 – 600 cm^{-1}. The thermal behavior of the sample was determined using the PerkinElmer Differential Scanning Calorimeter DSC 4000. The degradation temperature and other related properties were determined using PerkinElmer Simultaneous Thermal Analyzer, STA 6000. FTIR and Thermal analysis showed no significant changes in the chemical structure and thermal property of the material after subjecting to gamma irradiation. The optical microscopy images of the Stereolithography (SLA) 3D Printed tensile specimen was acquired and analysed using the Keyence Digital Microscope model VHX 7000.

Development of a machine for the manufacture of micro-optical lens and layered geometric forms of chalcogenide

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Micro lenses, signal paths and other products of complex geometry made of chalcogenide glass (for example, As2S(Se)3, As(Sb,Ge)-S(Se)-I(Br,Cl)) are widely applied in different areas to fulfill different functions. The use of additive manufacturing technologies for the manufacture of such products makes it possible to set high quality standards, as well as have mass production and low cost of production of products and almost complete waste-free production. In this paper developed an installation for the production of lenses and other products of complex geometry from chalcogenide glass by extruding a molten glass onto a prepared surface. The installation also allows you to create lenses of various geometric shapes. The installation consists of a three-axis robot, a computer vision system and a sealed chamber. A vision system with a trained neural network detects predetermined surfaces for applying glass and implements video tracking of surfaces online.

The three-axis robot extrudes the molten glass according to the coordinates of the surface to be applied calculated from video tracking. A sealed chamber protects the installation operator from harmful gases released from the molten glass. The developed prototype of the installation made it possible to create experimental optical sensors operating in the near and middle region of electromagnetic radiation.

This research work was supported by the Academic Excellence Project 5-100 proposed by Peter the Great SPbPU “Development of glassy and composite materials for biosensors and smart medicine devices”

WS2-Nanocharacterization & I3D	
16:30-16:45 16:45-17:00	**INVITED(V)** **R. Arenal, U. Zaragoza, Spain** In-situ TEM Studies on Low Dimensional Nanomaterials
17:00-17:15 17:15-17:30	**INVITED (V)** **V. Constantoudis NCSR Demokritos, Greece** The challenge of nanocomplexity
17:30-17:45 17:45-18:00	**INVITED (V)** **Vasileios Koutsos, The University of Edinburgh, United Kingdom** Microbubble Agents for Biomedical Applications: Focus on NanoMechanics and the NanoShell
18:00-18:15	**EU PROJECT (V)** **Sophie M Briffa, University of Birmingham, UK** Material Characterisation in the NanoScale: The value of standard methods and their transferability
18:15-18:30	**M. R. Koblischka Saarland University Germany (V)** Superconducting nanowire networks and the paramagnetic Meissner effect.
18:30-18:45	**E. G. Deze API Europe, Athens, Greece (L)** Mechanical Properties & Microstructural Investigation of Nanocellulose Enriched Cementitious Materials Cured in Aggressive Environments
18:45-19:00	**P. Ketikis National Technical Univ. of Athens, Greece (V)** The effect of graphene oxide on thermomechanical and permeability properties of poly(dimethyl siloxane) composites
19:00-19:15	**L. Burr Swiss Center for Electronics and Microtechnology (CSEM), Switzerland (V)** Hydrophobicity of nanomaterials measurements for risk assessment

In-situ TEM Studies on Low Dimensional Nanomaterials

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In-situ transmission electron microscopy (TEM) is a very powerful and useful technique to investigate the properties of nanomaterials, even to modify them. Importantly, the structural information at the sub-nanometer scale (even at the atomic level) can be obtained during the measurements in parallel [1-6].
In this contribution, I will present the TEM in-situ possibilities that we have via some examples going from the thermal reduction of the graphene oxide (GO) [5], the transport measurements of this material [6] and the transformation of different low-dimensional carbon-based nanomaterials [3, 4, 7]. These works illustrate the rich information that can be obtained via this kind of experiments and their interest for studying such nanomaterials. [8]. This detailed knowledge is essential for better understanding the outstanding properties of such materials.

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[6] S. Hettler, M. Pelaez-Fernandez, D. Sebastian, A.M. Benito, W.K. Maser, R. Arenal, to be submitted.
[7] M. Pelaez-Fdez, C. Ewels, A. Stergiou, D. Sebastian, N. Tagmatarchis, R. Arenal, To be submitted.
[8] Research supported by the Spanish MINECO (MAT2016-79776-P, AEI/FEDER, EU) and European Union H2020 programs “Graphene Flag-ship” (785219, 881603), “ESTEEM3” (823717) and Flag-ERA GATES (JTC-PCI2018-093137).

The challenge of nanocomplexity

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The big bang of nanofabrication techniques from the narrow area of electronics to the wider applications in energy, health and environment areas has been accompanied with a change in the geometrical characteristics of nanostructures. From the well-defined lithographic patterns used largely in semiconductor manufacturing, we have moved to more complex geometries to enhance surface properties and functionalities. These surfaces morphologies range from the almost periodic self-assembled nanostructures to the more random biomimetic morphologies usually characterized by hierarchical organization and multiscale structures. However, despite the extensive use of such complex nanostructured surfaces, a well-founded and concise mathematical characterization and metrology is still missing undermining their quantitative evaluation and large-scale production.
The aim of this talk is to address the challenge of nanocomplexity with emphasis on the mathematical characterization and metrology. The key idea is to put this challenge in the perspective of the complexity science and get inspiration by its mathematical concepts and methods.
In the first part, we will show plenty of real-world examples to identify the specific appearances of nanocomplexity in microscopy images. Then we will summarize the current approaches to their analysis found in recent literature. In the second part, we will elaborate two mathematical routes to the characterization of spatial nanocomplexity based on the broken symmetry concept. The first quantifies the complexity of a nanosurface by the deviation of its morphology from the average symmetry case (fully periodic and fully random) using entropy and information concepts. In the second, the focus is shifted to the scaling symmetry and an alternative to the multifractal formalism is proposed to provide robust and reliable measurements of multifractal spectra of nanosurfaces. Several applications will be presented in plasma treated polymer surfaces to reveal the benefits and limitations of both methods while emphasis will be given on their link to surface functionality.

Material Characterisation in the NanoScale: The value of standard methods and their transferability

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In the field of nanotechnology, characterisation plays a crucial role in understanding the behaviour, fate and toxicity of nanomaterials (NMs). An extensive range of characterisation techniques exist however there are several considerations that one should make before deciding which technique to use. Characterisation needs to be thorough and the technique chosen should be well-suited to the physical or chemical property to be determined, the material being analysed and the medium in which it is present. Therefore, guidelines on choosing appropriate techniques provide significant benefits to the scientific community. Furthermore, the instrument operation and methodology need to be well-developed and clearly understood by the user to avoid data collection errors. Any discrepancies in the applied method or procedure can lead to differences and poor reproducibility of obtained data. Results obtained from analytical characterisation interlaboratory comparisons studies within the H2020 ACEnano project have revealed the importance and benefits of detailed standard operating procedures (SOPs), best practice updates, user knowledge and measurement automation. Hence highlighting the value of developing reliable protocols and SOPs that are easily accessible and available for the scientific community. Additionally, once available these protocols and SOPs can be used and adapted for different fields as nanotechnology characterisation techniques are continuously being tailored for other disciplines.
One such important area to consider, particularly in the current pandemic, is virology. Nanotechnology techniques allow for faster, broader, quantitative characterisation of viruses and their interaction with NMs for the purposes of behaviour understanding and the development of treatments. The literature has shown that although the use of nanotechnology characterisation techniques within the field of virology is growing, there is still a great deal of potential to implement further techniques, particularly in dynamic or time-resolved experiments involving the interaction between NPs and viruses.

Superconducting nanowire networks and the paramagnetic Meissner effect

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Superconducting, ceramic high-T_c nanowire network fabric samples or fiber mats were fabricated using electrospinning or solution blow-spinning. Samples of $Bi_2Sr_2CaCu_2O_8$ (Bi-2212), $YBa_2Cu_3O_7$ (YBCO) and $GdBa_2Cu_3O_7$ (GdBCO) were fabricated applying both techniques. In all cases, we obtain fiber mats consisting of individual nanowires with very long lengths (up to 100 µm) and nanowire diameters ranging between 150 and 500 nm. To characterize the superconducting properties, SQUID measurements of the *M* vs. *T* and *M* vs. *H* were performed. The *M*-*H* magnetization loops reveal the granular, polycrystalline nature of the nanowires. In the Bi-2212 samples, we find a diamagnetic moment being overlaid on the superconducting signal, whereas in YBCO and GdBCO, a paramagnetic moment is present, which is very strong in GdBCO, so that always a positive *M*-*T*-signal is recorded. Having studied a large number of such fiber mat samples, we find that only the YBCO nanowire fiber mats exhibit the so-called paramagnetic Meissner effect (PME), whereas the other materials do not show this effect. The PME in the YBCO nanowires is found to be similar to that of artificially granular YBCO thin films, and is present only in weak magnetic fields. At higher applied magnetic fields, the samples are found to behave fully in the archetypal way. In this contribution, we give an explanation for this observation, regarding the current flow through the nanowires, the distinctly different current densities and the vortex dimensionality of the various materials (Bi-2212, YBCO and GdBCO) at elevated temperatures close to the superconducting transition temperature, T_c.

Mechanical Properties & Microstructural Investigation of Nanocellulose Enriched Cementitious Materials Cured in Aggressive Environments

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During the last years, incorporation of nanoadditives into concretes has been increasingly widespread thanks to their unique physicochemical properties which enable both nano- and micromechanical improvement of cement pastes. It has been well established that besides increasing concretes strength, refinement of pore size occurs causing a significant reduction in total porosity values and improvement in specimens durability. The present work aims at the analysis and performance evaluation of nanocellulose (CN) enriched Ultra High Durable Concretes (UHDC) exposed in aggressive environmental conditions (i.e. chemical attack - XA environmental exposure class). To that aspect, two reference UHDC materials containing crystalline admixtures and steel fibers were compared with mixes holding also cellulose nanocrystals (CNCs) and cellulose nanofibrils (CNFs) into their structures. In all cases, CN loading remained constant and equal to 0.15%wt (by %wt of cement amount). Preliminary results from compressive and flexural strength tests confirm that the incorporation of NCs into concrete mixtures can develop materials with enhanced mechanical properties. Additionally, microstructural analysis results suggest that the use of CNs can lead to the production of concretes with advanced textural and morphological characteristics and therefore widen their application prospects to aggressive environmental conditions.

The effect of graphene oxide on thermomechanical and permeability properties of poly(dimethyl siloxane) composites

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Graphene oxide (GO) nanoplatelets have already been used in preparation of polymer nanocomposites to improve mechanical, thermal and other performances of the reinforced materials.
In this study, the effect of graphene oxide (GO) on the properties composites with hydroxyl-terminated poly(dimethylsiloxane) (PDMS) matrices, prepared by solution mixing using tetrahydrofuran (THF) as a solvent were examined. Viscosity measurements during the vulcanization reaction using a Brookfield viscosimeter revealed that GO increases the viscosity of the system, in comparison with the unreinforced PDMS, proportionally to its concentration. The calculation of D and G bands ratio (I_D/I_G) at 1350 and 1580 cm^{-1} respectively, using RAMAN spectroscopy, showed more defects in graphene nanoplatelets incorporated in the PDMS nanocomposites. By Differential Scanning Calorimetry (DSC), slight decrease in glass transition and melting temperatures of PDMS was observed. The thermal stability of composites was significantly improved, especially at higher GO concentrations (0.5 and 1 phr), as it was detected by thermogravimetric analysis (TGA). Also, the tensile strength of the composites was enhanced, up to 113%, for samples reinforced with 1 phr GO. The elongation at break was increased, whereas no effect on the modulus of elasticity was observed. A decrease in oxygen permeability of 38% and 15% was measured in membranes made of composites containing 0.5 phr and 1 phr GO respectively. The increase in swelling after immersion of composites in toluene was explained by the fact that this phenomenon is not only related with the crosslinking density of the elastomer but also with the increased absorption properties of GO particles, due to the sonication treatment in the THF during the preparation process of the composite, might contribute to this effect.

Hydrophobicity of nanomaterials measurements for risk assessment

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The current increase of nanomaterial usage in industry fuelled by the race to miniaturization and performance improvements raises concerns on the potential risks associated with nanomaterials. The lack of industry-friendly risk assessment methods slows the implementation of such technologies leading to important financial losses for companies. Among the many properties of nanoparticles affecting their risk profile, such as size, concentration, composition or solubility, hydrophobicity has been identified in the nanosafety research community as one of the key properties to be characterized.

In the frame of the European ACEnano project, CSEM is developing innovative characterization techniques to describe the hydrophobicity of nanoparticles. Here we present the assessment of hydrophobicity of polystyrene based nanoparticles with various surface functionalizations. We could successfully show that with a new surface-based method, hydrophobicities can be characterized and compared, which in turn can be used to develop a qualitative comparison chart for nanoparticles.

I3D	
16:30-16:45 16:45-17:00	**INVITED** **Bandar AlMangour, Saudi Arabia Basic Industries Corporation, Saudi Arabia** Strengthening of stainless steel by reinforcement addition and grain refinement during additive manufacturing
17:00-17:15 17:15-17:30	**INVITED** **Fedor Antonov, Anisoprint, Russia** Anisoprinting technology: continuous fiber 3D printing for manufacturing of optimal composites
17:30-17:45	**Huachao Mao Purdue University, USA** A novel resin vat design to accelerate the resin flow in quasi-continuous vat photopolymerization
17:45-18:00	**EU PROJECT (L)** **Dr Ilise L Feitshans JD and ScM and DIR** Emerging Laws for 3D Product Design
18:00-18:15	**Dror Danai, Xjet Ltd., ISRAEL** XJET NanoParticles Jetting Ceramic and metal additive manufacturing technologies & solutions
18:15-18:30	**Konstantinos A. Sierros, West Virginia University, USA** 3D printing of smart building blocks for space soft robotics
18:30-18:45	**Konstantinos A. Sierros West Virginia University, USA** 3D Printing of Lithium Solid State Batteries

Strengthening of stainless steel by reinforcement addition and grain refinement during additive manufacturing

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This study examines the role of micro- and nano TiC and TiB_2 added to 316L stainless steel fabricated by the selective laser melting (SLM) process, an emerging additive manufacturing technology, in the microstructural evolution, mechanical properties, and tribological performance. It was found that the microstructure and mechanical properties of the SLM-processed nanocomposites were sensitive to the reinforcement content and also the size. Directionally fine cellular dendrites and columnar grains formed during the fast solidification in SLM-processed stainless steel. Interestingly, the addition of ceramic particles in the steel matrix significantly reduced the cellular and grain sizes after solidification and also disrupted the established directional structures, particularly for nanoscale reinforcement. The composite, particularly with nanoscale reinforcements, also exhibited greater compressive yield strengths and tribological performance than unreinforced steel, mainly because of the combined effects of grain-boundary strengthening and Orowan strengthening. The strengthening effect was well described by the Zener pinning model. The compressed surfaces suggest that reinforcement particles hinder crack propagation, and the reinforcement particles distribution was critical in improving the mechanical properties. The SLM process can tailor the microstructure across a rather limited length scale; hence, to better control the mechanical properties of the resulting products, compositing the relevant feedstock powder is a highly attractive strategy for developing components with novel structures and unique properties.

Anisoprinting technology: continuous fiber 3D printing for manufacturing of optimal composites

Fedor Antonov

CEO (Anisoprint)

9 avenue des Hauts Fourneaux,

Esch-sur-Alzette L-4362, Luxembourg-Russia

Anisoprinting is a technology of continuous fiber 3D printing for manufacturing of optimal composites. Polymers reinforced with continuous fibers are 30 times stronger than pure plastic, 2 times stronger and lighter than aluminum. Anisoprint's open system allows choosing custom fiber laying trajectories, manufacturing composites of the complex shapes, with unlimited materials choice, cheaper and easier to produce than metal or non-optimal 3D printed composites.

A novel resin vat design to accelerate the resin flow in quasi-continuous vat photopolymerization

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Continuous Vat photopolymerization, such as Continuous Liquid Interface Production (CLIP) and High Area Rapid Prototyping (HARP), has achieved a remarkable high Additive Manufacturing (AM) speed (~500 mm/hour), which transforms the AM to rapid manufacturing. However, the printing speed dramatically slows down for viscous resin and 3D objects with wide cross sections, since the viscous resin can be effectively replenished through a narrow (20um ~ 50um) oxygen inhibition layer. We propose a novel oscillating resin vat design to accelerate the resin flow while the building platform lifts continuously. The resin vat has channels with milli-meter scale depth to quickly replenish the resin. The rest of the resin vat is filled with Polydimethylsiloxane (PDMS) which permeates oxygen to enable a liquid photopolymerization-inhibited resin layer to enable continuous photopolymerization. As a proof of concept, we experimentally validated that the proposed resin vat could continuously print solid objects with wide cross-section (3000 mm^2). We theoretically derived a model to predict the proposed throughput as a function of the process parameters: resin curing property, vat geometry, and curing light intensity. We also revealed that the vat-part suction force was greatly reduced compared with that of a resin vat without channels, which mitigated the printing failures and part deformation.

XJET NanoParticles Jetting Ceramic and metal additive manufacturing technologies & solutions

Mr. Dror Danai *Xjet Ltd.*
2 Oppenheimer Street, Rehovot, ISRAEL

With a decade of research behind it, the NPJ technology enables the production of metal or ceramic parts with the same ease and versatility of inkjet printing without compromising throughput or quality. The presentation is intended for audience and visitors that are seeking to be familiar with the most up-to-date technology enhancement.
Our trailblazing NPJ technology is the talk of the AM industry. XJet's NanoParticle Jetting™ (NPJ) technology enables the production of metal and ceramic AM parts featuring unprecedented levels of detailing, finish and accuracy, while delivering physical, geometric and operational advantages. Leveraging NPJ's key features of stochastic nanoparticles, ultra-thin layers and simultaneous jetting, XJet delivers on the AM promise by creating "complexity free" high-quality parts with virtually unlimited geometries in an operationally efficient manner.

Thursday 9th July

KEYNOTE

11:00-11:30	**KEYNOTE (V)** **Prof. George Maliaras, Cambridge University, UK** Electronics on the Brain

Electronics on the Brain

G. Malliaras

Department of Engineering, University of Cambridge, Cambridge, UK

One of the most important scientific and technological frontiers of our time is the interfacing of electronics with the human brain. This endeavour promises to help understand how the brain works and deliver new tools for diagnosis and treatment of pathologies including epilepsy and Parkinson's disease. Current solutions, however, are limited by the materials that are brought in contact with the tissue and transduce signals across the biotic/abiotic interface. Recent advances in organic electronics have made available materials with a unique combination of attractive properties, including mechanical flexibility, mixed ionic/electronic conduction, enhanced biocompatibility, and capability for drug delivery. I will present examples of novel devices for recording and stimulation of neurons and show that organic electronic materials offer tremendous opportunities to study the brain and treat its pathologies.

WS4	
11:30-12:00	**INVITED (V)** **Dr. Francesco De Angelis, Italian Institute of Technology, Italy** Plasmonic nanostructured surfaces for bio-interfaces and sensing of living cells
12:00-12:15 12:15-12:30	INVITED (V) **Dr. Paschalis Gkoupidenis, Max Planck Institute for Polymer Research, Germany** Electrolyte-gated transistors for neuromorphic electronics
12:30-12:45 12:45-13:00	**INVITED** **G.M. Farinola, Università degli Studi di Bari, Italy** Photoactive materials for bioelectronics from photosynthetic microorganisms

Plasmonic nanostructured surfaces for bio-interfaces and sensing of living cells

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Genova, Italy y

The ability to interact with living cells and to monitor their status plays a pivotal role in neuroscience, pharmacology and cell biology. In the last years, we deeply investigated both theoretically and experimentally the interactions of 3D nanostructured surface sensors with living cells such human neurons and cardiomyocytes. The aim is to make an effective interface between the intracellular compartment and different class of nano-sensors including optical sensors (plasmonic enhanced spectroscopies), electrodes and nano-needles for intracellular delivery or sampling. We developed a method based on plasmonic generation of nano-shockwaves for opening transient nanopores into the cell membrane. After the membrane poration the tip of the sensor is in direct contact with the intracellular compartment thus enabling intracellular investigations which include Raman traces of biomolecules, electrical recording of action potentials of human neurons and cardiomyocites, and controlled delivery of single nanoparticles into selected cells. Recently we introduced the concept of planar meta-electrodes and we combined these technologies with CMOS multi-electrode arrays. We demonstrated the possibility of non-invasively testing the effect of relevant drugs on human cells with particular regard of cardio-toxicity that is a fundamental step before the clinical trials. Due to its robustness and easiness of use, we expect the method will be rapidly adopted by the scientific community and by pharmaceutical companies. In fact, the field suffers the lack of reliable approaches for pharmacological screening of drugs devoted to the central nervous system. Also, we will take this opportunity to give a short overview of different optical biosensors we are currently developing such as single molecule Raman Sensors, DNA sensors, and novel technologies for protein sequencing.

Electrolyte-gated transistors for neuromorphic electronics

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Neuromorphic devices and architectures offer novel ways of data manipulation and processing, especially in data intensive applications. At a single device level, various forms of neuroplasticity have been emulated over the past years, mainly with inorganic devices. The implementation of neuroplasticity functions with these devices also enabled applications at a circuit level related to machine learning such as pattern recognition. Although the field of organic-based neuromorphic devices and circuits is still at its infancy, organic materials may offer attractive features for neuromorphic engineering. Over the past years for example, a few simple neuromorphic functions have been demonstrated with biological substances and bioelectronic devices.

Here, various neuromorphic devices will be presented that are based on organic mixed conductors, materials that are traditionally used in organic bioelectronics. A prominent example of a device in bioelectronics that exploits mixed conductivity phenomena is the organic electrochemical transistor. The device operation in common electrolyte permits the definition of spatially distributed multiple inputs at a single device level. The presence of a global electrolyte in an array of devices also allows for the homeostatic or global control of the array. Global electrical oscillations can be used as global clocks that phase-lock the local activity of individual devices in analogy to the global oscillations in the brain. Finally, “soft” interconnectivity through the electrolyte can be defined, a feature that paves the way for parallel interconnections between devices with minimal hardwired connections.

Photoactive materials for bioelectronics from photosynthetic microorganisms

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Photosynthetic microorganisms can be envisaged as a source of active materials for bio-optoelectronic devices for photoconversion.

We have demonstrated the use of the Reaction Center (RC) from the photosynthetic bacterium *Rhodobacter sphaeroides* R26 in bioelectronic and photoelectrochemical devices. Photosynthetic Reaction Centers (RCs) are photoenzymes capable to convert solar energy into charge separated states with efficiency close to 100%. We have first reported the highly selective covalent functionalization of the bacterial RC with several classes of tailored molecular fluorophores which act as antennas to enhance its light harvesting capability. We have also built up supramolecular architectures combining multiple enzymes assembled with tailored linkers, which are able to perform manifold functions. Finally, we have developed protocols for addressing the RC on thin films of molecular or polymeric semiconductors or on metal electrodes by covalent or weak collective interactions, obtaining RC-sensitized electronic and electrochemical devices. Biomimetic polymers, such as polydopamine mimics of melanines, have also been used as efficient electronic interfaces of RC with electrodes in photoelectrochemical cells.

Our study discloses new concepts for the generation of bio-hybrid materials for sunlight photoconversion and for light-responsive bioelectronics, from the combination of photosynthetic bacterial enzymes with tailored functional molecules.

F.Milano, A. Punzi, R. Ragni, M. Trotta, G.M. Farinola, *Adv. Funct. Mater.* **2020**, *29*, 180551

WS5	
11:30-12:00	**INVITED (V)** **A. Di Bartolomeo University of Salerno, Italy.** Pressure, temperature and radiation effects on back-gate transistors based on layered 2D materials
12:00-12:15 12:15-12:30	**INVITED (V)** **A. Stergiou, National Hellenic Research Foundation, Greece** Covalent functionalization of exfoliated MoS2 with organic motifs for the selective recognition of ions and molecules
12:30-12:45	**O. Kochanowska, University of Warsaw, Poland (V)** Laser-pulse-driven control of Landau-Zener transitions in graphene
12:45-13:00	**J. Derlikiewicz, University of Warsaw, Poland (V)** Vortex-like current density structures in graphene subjected to a bicircular laser field

Pressure, temperature and radiation effects on back-gate transistors based on layered 2D materials

A. Di Bartolomeo[1,2,3], E. Faella[1], F. Giubileo[2], A. Grillo[1,2], L. Iemmo[1,2], A. Pelella[1,2], F. Urban[1,2,3]
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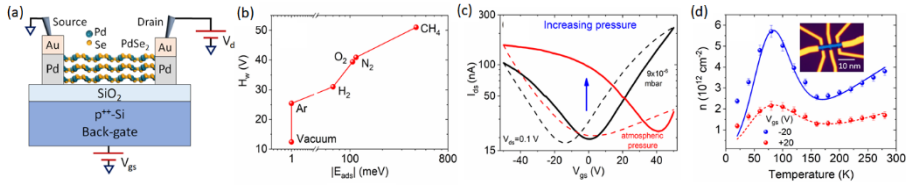
Two-dimensional materials are highly attractive in electronic devices for the tunable bandgap and mobility, the strong interaction with light, the easy formation of van der Waals heterojunctions, the mechanical robustness and the chemical stability. In this study, we deposit nanosheets of MoS_2, WSe_2, $PdSe_2$ or GeAs onto SiO_2/Si substrates to fabricate back-gate field-effect transistors and investigate the effects of gas pressure, temperature and electron irradiation. We show that gas adsorption enhances the hysteresis observed in the transfer characteristics, while gas pressure controls the polarity of the devices. The dominant n-type behavior in a high vacuum and the sharp-edge geometry enable field emission current, which we extensively characterize under different conditions. We investigate the temperature dependence of the electrical conductivity and we report an anomalous peak in the carrier density per area at low temperature, that we interpret as the manifestation of a 2D conduction phenomenon in multilayer nanosheets. Finally, we show that electron beam irradiation degrades the channel conductivity, yet it can be exploited to control the Schottky barrier at the metal electrodes and to reduce the contact resistance.



(a) Back-gate transistor.
(b) MoS_2 hysteresis vs gas adsorption energy.
(c) $PdSe_2$ transfer curves vs pressure.
(d) GeAs carrier density vs temperature.

Covalent functionalization of exfoliated MoS_2 with organic motifs for the selective recognition of ions and molecules

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Molecular recognition is an important mechanism of nature in order to maintain the selectivity of numerous processes taking place at the nanoscale. Static molecular recognition is represented by the keyhole-key scheme, namely host-guest complexes with a 1:1 stoichiometry, where molecular design enables direct intermolecular interactions via coordination, van der Waals forces, ??? hydrophobic attractive forces, H-bonding etc. Undoubtedly, crown ethers paved the way towards the synthesis of artificial molecular recognition architectures, while the rise of nanomaterials empowered the design of functional hybrid materials with nanoscale precision. In this context, we utilize crown ethers as robust candidates for the highly selective host-guest recognition of alkali metal cations. Their covalent incorporation on the surface of exfoliated molybdenum disulfide (MoS_2) facilitates a uniform allocation on a 2D surface with exceptional charge transport properties. An array of complementary spectroscopic, thermal and electrochemical techniques is applied for the characterization of the newly synthesized hybrid covalently bound ensembles. Host-guest complexation is probed by redox techniques and the potential as a sensitive and selective electrochemical sensor is evaluated.

Acknowledgements: This research is co-financed by Greece and the European Union (European Social Fund- ESF) through the Operational Programme «Human Resources Development, Education and Lifelong Learning 2014-2020» in the context of the project “Chemically modified MoS_2 with organic recognition motifs as electrochemical sensors for the selective detection of ions and (bio)molecules” (MIS 5048201).

Laser-pulse-driven control of Landau-Zener transitions in graphene

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Graphene – a two-dimensional monolayer of carbon atoms arranged in honeycomb lattice – is a rising star in nanotechnology. This relatively new material exhibits extraordinary mechanical, electronic and optical properties, which attracted significant attention in the world of science. Owing to its linear energy dispersion at Dirac points, graphene is called “semi-metal” and provides a promising model to test electron dynamics in conducting materials under the illumination of strong laser field.

Interaction of strong laser field with graphene reveals interesting phenomena in non-perturbative regime. Our aim is to analyse such effects in graphene when subject to linearly polarised laser pulses. In this case, we calculate numerically electron excitation probability as a function of laser pulse amplitude. We demonstrate that the electron can undergo non-adiabatic transitions from the valence to the conduction band. These interband transitions are well described by Landau-Zener theory. By modifying laser pulse parameters, such as envelope shape or pulse duration, one can control Landau-Zener transitions, i.e., steer electrons dynamics in graphene. We demonstrate, for instance, that for long laser pulses intraband motion is observed – electrons stay adiabatically in the valence band, whereas for short pulses adiabaticity is not preserved and non-adiabatic transitions to the conduction band occur. As we show, this happens at the avoided crossings of quasi-energy surfaces, which arise within the Floquet theorem.

Vortex-like current density structures in graphene subjected to a bicircular laser field

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Graphene is considered to be one of the most versatile materials in solid-state physics. In recent years it has become one of the main research topics in both theoretical and experimental physics, mainly thanks to its large number of potential applications. What is perhaps the most interesting about this novel material are its electrical characteristics, which are directly linked to many of graphene’s extraordinary properties. Due to its unique atomic structure, the electrons in the vicinity of the Dirac points can easily move between valence and conduction bands at extremely high velocities without a significant chance of scattering; thus saving energy, which would typically be lost in other non-zero band gap conductors.

In this research, the behaviour of the electrons near the K points in graphene subjected to a bicircular laser field was analyzed. The current density was calculated from the Dirac-Weyl equation for low-energy excitations in monolayer graphene using the Floquet theory combined with Fourier decomposition, and the total current was obtained. As a result, vortex-like current structures on the surface of graphene were observed and interpreted. It was also postulated that this outcome may lead to the occurrence of other non-linear effects such as high harmonic generation.

WS4

	WS4
14:00-14:15	**INVITED (V)**
14:15-14:30	**Vasiliki Giagka , Delft University of Technology, Netherlands** Engineering long-lasting and spatially selective active neural interfaces for biolectronic medicine
14:30-14:45	**INVITED (V)**
14:45-15:00	**Eleonora Macchia, Åbo Akademi University, Finland** Selective Single-Molecule Detection of clinically relevant biomarkers with an Organic Transistor
15:00-15:15	**INVITED (V)**
15:15-15:30	**Prof. Beatrice Fraboni, University of Bologna, Italy** Morphology and mobility as tools to control X-ray sensitivity in organic thin-films
15:30-15:45	**D. Kourkoulos, Coatema Coating Machinery GmbH, Germany** Nanocellulose Coated Paper as Substrates for a sustainable, quantitative and environmentally friendly bio sensing platform
15:45-16:00	**J. Morgado Instituto de Telecomunicações, , Portuga**l Opportunities and Challenges in the Use of Conductive Polymeric Scaffolds for Stem Cell Culture
16:00-16:15	**Dimitrios A. Koutsouras Max Planck Institute for Polymer Research, Mainz, Germany (V)** Microelectrodes coated with conducting polymers for bioelectronics: scaling properties and biosensing
16:15-16:30	**J. M. Marmolejo-Tejada Pontificia Universidad Javeriana, Colombia, (V)** Partially-Oxidized Phosphorene-Based Sensors and Surface Oxidation Effects
16:30-16:45	**S.D. Psoma The Open University, U.K. (V)** Computational analysis and design of microchambers for multianalyte aptamer-based biosensor applications
16:45-17:00	**S. Grammatikos, Aristotle University of Thessaloniki, Greece** Synthesis and characterization of biofunctionalized AuNPs for future use in screen-printed electrochemical immunosensors
17:00-17:15	**Kalligosfyri Panagiota, University of Patras, Greece** Gold nanoparticle-based biosensor for rapid liquid biopsy applications
17:15-17:30	**M. C. Suster, University of Warsaw, Poland** Plasmonic nanoaperture arrays for biosensing applications

Engineering long-lasting and spatially selective active neural interfaces for biolectronic medicine

Vasiliki Giagka[1,2]

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In a world where medicine is becoming more personalised the promise of Bioelectronic Medicine is that tiny implants will deliver energy in the form of electrical impulses, replacing pharmaceuticals, their conventional chemical counterparts. But how can we develop such tiny smart and autonomous implants that (need to) seamlessly interact with the tissue and live in the body for decades [1]? How can we protect all the components in such an implant while still maintaining the small form factor and essential flexibility [2]? How can we design electronics such that they remain better protected in such a harsh environment [3]? How can we ensure autonomy under the above restrictions [4]? Eventually, how can we make our medicine more precise, i.e. increase the specificity at which we interact with the tissue [5, 6]? This talk will aim to address these questions and present an overview of how to engineer long-lasting and spatially selective active neural interfaces.

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Selective Single-Molecule Detection of clinically relevant biomarkers with an Organic Transistor

Eleonora Macchia,[1*] Rosaria A. Picca[2] Kyriaki Manoli,[2] Nicola Cioffi,[2] Cinzia Di Franco,[3] Gaetano Scamarcio,[4] Gerardo Palazzo,[2,4] Fabrizio Torricelli,[5] Ronald Österbacka,[1] & Luisa Torsi,[1,2,4]

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The *US National Institute of Health* defines biomarkers *as molecules that can be objectively measured and evaluated as indicators of normal or disease processes and pharmacologic responses to therapeutic intervention*. Among the plethora of biomarkers, the sensitive detection of proteins is of paramount importance in a number of clinical fields.[1] The clinical use of protein biomarkers as indicators of the onset of pathological states requires the measurement of low concentrations of proteins in complex samples. Attempts to develop ultra-sensitive assays for the detection of protein biomarkers have been done by several groups in the last few years. Although in the last decade many approaches to achieve ultra-sensitive detection have been developed, most of them require complicated assay set-ups, hindering their adoption in point-of-care applications. In this perspective, Electrolyte-Gated Field-Effect-Transistors (EG-FETs) [2-4] with a bio-functionalized gate electrode, appear as very promising biosensing platforms. The EG-FET device herein presented, able to operate in physiologically relevant fluids such as blood serum and saliva, will set the ground to a major revolution in biosensing applications for early clinical detection.

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Morphology and mobility as tools to control X-ray sensitivity in organic thin-films

Beatrice Fraboni
Department of Physics and Astronomy, University of Bologna, Italy)

Organic semiconductor materials exhibit a great potential for the realization of large-area solution-processed devices able to directly detect high-energy radiation. However, only few works investigated on the mechanism of ionizing radiation detection in this class of materials, so far. In this work we investigate the physical processes and parameters behind X-ray photoconversion in organic thin films.
We employ bis-(triisopropylsilylethynyl)-pentacene thin-films deposited by bar-assisted meniscus shearing as direct X-ray detectors. The thin film coating speed and the use of bis-(triisopropylsilylethynyl)-pentacene:polystyrene blends are explored as tools to enhance the detection capability of the devices, by tuning the thin-film morphology and the carrier mobility . We succeed not only in tuning and enhancing the sensitivity of the detectors but also in studying the role of the electrically active defects related to the grain boundaries in the detection process. We demonstrate that carrier mobility and thin-film morphology (i.e., number and size of grain boundaries) are the two main parameters affecting the photoconductive gain process and the carrier trapping effects, that is, the physical processes that explain why thin organic films can directly detect high-energy radiation. The so-obtained detectors reach a record sensitivity of $1.3 \cdot 10^4$ $\mu C/Gy \cdot cm^2$, the highest value reported for organic-based direct X-ray detectors and a very low minimum detectable dose rate of 35 µGy/s [1]. Thus, the employment of organic large-area direct detectors for X-ray radiation in real-life applications can be foreseen.
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Nanocellulose Coated Paper as Substrates for a sustainable, quantitative and environmentally friendly bio sensing platform

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Printed electronics are one of the fastest growing technologies in the world. Paper and plastics are two key substrates for the development of future flexible electronic devices. As opposed to devices fabricated onto plastic substrates, paper-based electronics, made from cellulose, would have several advantages like low cost, and recyclability; and are expected to have a significant impact in the reduction of the environmental impact of "electronic waste".
Unfortunately, the surface properties of conventional paper are not suitable for printed electronics. Recent studies however have shown that the application of a nanocellulose layer helps to overcome this issue and thereby meet the requirements for printed electronics (e.g. by enhancing the printability of the substrate). In the Horizon 2020 funded project GREENSENSE Coatema, together with the other project partners develops a sustainable, quantitative and environmentally friendly bio sensing platform for Drug-of-Abuse analysis onto a nanocellulose based substrate. The focus of Coatema's work in this project is on the coating of a homogenous nanocellulose layer with the required surface properties and the upscaling of this process up to a pilot production. Processing nanocellulose and to obtain homogeneous defect free layers is quite challenging. The unexceptionally high viscosity and thixotropic behavior of nanocellulose based solutions makes it difficult to deposit this material with standard coating methods. Furthermore, another crucial aspect is the high solvent content of the typical nanocellulose solution (between 99 and 95%), causing very high demands for the drying process. We will present our results towards the fabrication of nanocellulose layers that can facilitate the application of paper substrates in printed electronics.

Opportunities and Challenges in the Use of Conductive Polymeric Scaffolds for Stem Cell Culture

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Neural stem cells or mesenchymal stem cells therapies have the potential to treat neurodegenerative diseases. In order to fully achieve that goal, we are developing novel conductive scaffolds that, by mimicking the extracellular matrix, can be used to support culture cells *in vitro* and control their fate.
We have been studying the fabrication of scaffolds with various topographies based on conjugated polymers for neural stem cells cultivation and/or differentiation using patterned devices [1]. We aim to assess the role of different materials and topographies on cells fate, with and without the application of electrical stimulus.
In this communication we report on our progress in the search for polymer and polymer blends-based films and fibers scaffolds, and their ability to sustain viable cell culture.

We acknowledge FCT financial support under the projects NEURON (PTDC/CTM-CTM/30237/2017), UIDB/04565/2020 and UIDB/50008/2020.

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Microelectrodes coated with conducting polymers for bioelectronics: scaling properties and biosensing

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Abstract: Conducting polymer coated electrodes have been widely used to bridge the gap between the worlds of electronics and biology due to their unique set of features. Their use in various applications, span the whole spectrum from neural stimulation and activity recording to drug delivery and biosensing. Nevertheless, their device physics is not yet fully understood. In that context, an experimental and systematic study based on sensing device impedance spectra, with and/or without the presence of biological tissue, is of great importance. In this work, with the use of impedance spectroscopy, we investigate the way that the impedance ratio of a biological cell layer to the measuring device, affects the recording ability of the latter. Various sized PEDOT:PSS (Poly(3,4-ethylenedioxythiophene):polystyrene sulfonate) coated electrodes are employed and the effect of their dimension to their performance is determined. A simple equivalent circuit is proposed to model the conducting polymer device, as well as the biotic/abiotic ensemble, and a scale law that leads to an impedance master curve is revealed. Finally, analytical expressions of the total impedance as a function of frequency are extracted. Overall, the study reveals a critical impedance ratio of the biological tissue to the sensor, which allows for efficient sensing of the integrity of the former. The results open new pathways for the realization of improved impedance-based biosensors with optimized sensitivity.

Partially-Oxidized Phosphorene-Based Sensors and Surface Oxidation Effects

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Label-free sensors capable of detecting low concentrations of biomolecular substances without inducing immune response would simplify experiments, minimize errors, improve real-time observations and reduce costs in probing living organisms. Due to their usually high electronic mobility and surface-to-volume ratio, two-dimensional (2D) materials are expected to enable the accurate detection and measurement of targeted biological markers (biomarkers) in nano-molar (nM) or pico-molar (pM) concentrations, through differentiable electronic signatures [1-3]. Notwithstanding the potential of phosphorene-based devices for sensing applications, their usability has been compromised by the material's fast degradation under ambient conditions. However, several approaches have been considered for improving the material's stability during long periods of time, such as the recently demonstrated partially-oxidized phosphorene (po-phosphorene) [4-5]. Here, we present a computational study of phosphorene-based field-effect gas sensors, using Density Functional theory (DFT) and Density-Functional-based Tight Binding (DFTB) methods coupled to non-equilibrium Green's Functions (NEGF) for characterizing their electronic transport properties at different surface oxygen concentrations, aiming to demonstrate their potential use in selectively detecting and measuring nitrogen species, as NO and NO_2.

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Computational analysis and design of microchambers for multianalyte aptamer-based biosensor applications

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This study presents different designs of microfluidic modelling and simulation of multianalyte microchambers for aptamer-based biosensor applications using fluorescence detection method. Each microchamber including the microchannels is the point of interest for the interactions with the target analyte and the optical detection. Their design and fluidic parameters are highly important for the performance of the biosensor by holding the immobilised aptamers onto their surfaces without leaching issues and with integration of the optical detection method by offering high sensitivity and repeatability. As a result, the shape, size and microchannel design and connections are vital parameters. In the present work, several combinations of different shapes of microchambers and microchannels are designed and simulated. Fluidic parameters such as average velocity, pressure, flow rates shear parameters are critically assessed at different cross-sections within the microchambers.

The rinsing behaviour with buffer solutions under certain pressure drops between the inlet and outlet microchannels are investigated. Another challenge in the design of the microfluidic unit of the multianalyte biosensor lies in the extraction of entrained air bubbles, which may be present after the filling process is completed, dramatically affecting the performance of the sensing element. Optimised design of the microchambers is selected based on optimal rinsing, minimum flow shear, avoidance of slow zones without reverse flows, relatively simple geometry, minimum static pressure drops and homogenous distribution of the different analyte targets. Steady and unsteady flow simulations were carried out using a commercial Computational Fluid Dynamics code and involved an extensive parametric analysis.

Synthesis and characterization of biofunctionalized AuNPs for future use in screen-printed electrochemical immunosensors

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Due to their unique properties and multiple surface functionalities, gold nanoparticles (AuNPs) have been widely used in various biomedical applications, such as biosensors/bioassays. In the present study, AuNPs were synthesized via Turkevich method and linked with Cysteamine (Cys-AuNPs), as well as via a modified-Turkevich method based on the use of Chitosan (Chit-AuNPs) instead of Trisodium Citrate as reducing/stabilizing agent. The created solutions were studied with UV-Vis absorption spectra measurements, in order to validate the plasmon resonance band of the AuNPs. The resulted AuNPs were also characterized via Atomic Force Microscopy (AFM) measurements after depositing them onto rigid substrates in terms of morphology, shape and size distribution, revealing the necessary properties so as to be used for further process. Following, they were biofunctionalized by biorecognition elements (antibodies) attached on either Cysteamine or Chitosan binding sites, for the purpose of using them as an immobilization platform in immunosensors. The construction of the proposed electrochemical immunosensors is based on the screen-printing technology for the patterning and deposition of the Working, Counter and Reference Electrodes (WE, CE, RE), with a goal of creating an innovative, low cost, disposable and effective electrochemical immunosensor system for various sensing applications.
Acknowledgement: This study has been funded by the H2020-DT-NMBP-08-2020 Project RealNano (www.realnano-project.eu)

Gold nanoparticle-based biosensor for rapid liquid biopsy applications

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Liquid biopsy offers a non-invasive, easy, quick and convenient alternative approach for early diagnosis of cancer and real-time monitoring of tumor progression. Liquid biopsies assess various biomarkers mainly represented by blood circulating tumor cells (CTC), circulating tumor DNA (ctDNA), circulating microRNAs and exosomes that are secreted by the tumors. Using body fluid samples, liquid biopsies may be the ideal approach for the detection of these biomarkers. The presence of circulating tumor DNA (ctDNA) or cell-free DNA (cfDNA), derived from tumors, in blood circulation is of major importance for early cancer detection, monitor tumor progress or diagnose the presence of activating mutations to guide treatment. The ability to detect ctDNA can serve as a liquid biopsy clinical application. In this project, a new gold nanoparticles-based DNA biosensor was developed for the detection of the most significant/common mutations in KRAS gene related to colorectal cancer in cell-free tumor DNA. Three major mutations and the normal allele of KRAS gene were detected by the biosensor. The biosensor was firstly optimized using synthetic DNA targets and was then applied to specific cell lines and blood serum samples. DNA and cell-free DNA were isolated from the samples, amplified, subjected to allele-discrimination reaction and analysed with the biosensor. This biosensor offers simplicity, as no expensive instrumentation is required, rapid analysis that is completed within 10 min, high detectability, specificity and reproducibility, while the detection is accomplished by naked eye.
"This research is co-financed by Greece and the European Union (European Social Fund- ESF) through the Operational Programme «Human Resources Development, Education and Lifelong Learning 2014-2020» in the context of the project "Gold nanoparticle-based biosensor for rapid liquid biopsy applications" (MIS 5047147)."

Plasmonic nanoaperture arrays for biosensing applications

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LSPR-based plasmonic biosensors are a class of nano-optical devices which utilize collective excitations of surface plasmons to detect presence of an analyte. Their remarkable sensitivity to refractive index change which occurs during surface binding events stems from a strong enhancement and localization of the electromagnetic field at the vicinity of various metallic nanoobjects.

In this study, large-area glass substrates with arrays of plasmonic nanoapertures were fabricated and investigated. To ensure homogeneity of the samples on an area of a few centimeters by a few centimeters, nanosphere lithography combined with e-PVD and mechanical exfoliation was used as an alternative to standard, area-limited and time-consuming methods like electron-beam or ion-beam lithography. Optical properties of the samples can be adjusted by altering the thickness of the metallic layer, diameters of the apertures or their relative position and arrangement. The overall quality and characteristics of the obtained structures were evaluated using SEM imaging, UV-VIS reflectometry and label-free sensing experiments.

WS5

	WS5
14:00-14:15	**KEYNOTE**
14:15-14:30	**Paul K Hurley, Tyndall National Institute. Ireland** Investigating the Interface between MoS_2 and Insulating Oxides
14:30-14:45	**INVITED**
14:45-15:00	**Dr. George Deligeorgis, FORTH IESL, Greece** Carbon Nano-Tube and Transition Metal Dichalcogenide smart electronics
15:00-15:15	**INVITED (V)**
15:15-15:30	**A. Krivosheeva Belarusian State University of Informatics and Radioelectronics, Belarus** Heterostructures of two-dimensional transition metal dichalcogenides: formation, ab initio modeling and possible applications
15:30-15:45	**Najeh Jisrawi, Centre for Advanced Materials Research, UAE** A study on the electronic properties of Graphene Nanoribbons using the Offset Logarithm function
15:45-16:00	**A. I. Velea, Delft University of Technology, The Netherlands** Soft, flexible and transparent graphene-based active spinal cord implants for optogenetic studies

Investigating the Interface between MoS_2 and Insulating Oxides

Paul K. Hurley[1], Emma Coleman[1], Gioele Mirabelli[1], Enrico Caruso[1], Farzan Gity[1], Peng Zhao[2], Pavel Bolshakov[2], Robert M. Wallace[2] and Chadwin D. Young[2]

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Two-dimensional van der Waal's bonded semiconductors exhibit energy gaps which span from semi-metals through to wide band gap semiconductors and as a consequence have potential applications in electron devices, photonics and sensors technologies [1]. In the area of insulating gate electron devices, the 2 dimensional structure of the semiconductor has the potential to result in near ideal semiconductor/oxide interface properties, which is one of the main factors motivating research into MOSFET and tunnel FET devices based on 2D channel semiconductors.

This presentation will focus on the application of impedance spectroscopy (100Hz to 1 MHz) to examine the electronic properties of Al_2O_3/MoS_2 capacitor structures [2-5]. The results are presented for thin channel (5-10 layers of MoS_2) top gated MOSFET structures as well as back gated MOS capacitor structures. The results and analysis indicates that the capacitance and conductance of the structures, as a function of voltage and ac signal frequency, can be used to quantify electrically active defects states at the Al_2O_3/MoS_2. An analysis of the Al_2O_3/MoS_2 impedance response, using fully physics based *ac* modelling, indicates that while defects in the Al_2O_3 still play a significant role, near ideal interface properties between Al_2O_3 and MoS_2 can be achieved,

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Carbon Nano-Tube and Transition Metal Dichalcogenide smart electronics

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Carbon nanotubes and more recently graphene and other two dimensional materials have emerged as a potential solution for new generation electronics. Their extreme form factor enable aggressive downscaling of related devices. However, as with any new technology the road to maturity is paved with challenges and a host of technological issues that need to be addressed before such technology performs comparably to current electronics. Furthermore, 2D materials are inherently sensitive to their surrounding making processing complex circuits a challenge.

The state of the art in electronics based on such technologies will be presented and the potential of each technology will be presented. We will finally focus on our approach to combine 2D and CNT materials to achieve the next generation sensors and analogue high frequency electronics for wireless smart applications.

Heterostructures of two-dimensional transition metal dichalcogenides: formation, *ab initio* modeling and possible applications

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Marseille, France

State-of-the-art technologies of fabrication of transition metal dichalcogenide monolayers like MeX_2, where Me = Mo, W; X = S, Se, Te, and their based heterostructures are considered. The results of theoretical modeling are analyzed and the possibilities of band gap engineering by means of strains, impurities, vacancies, various layer stacking and combination of different materials are presented. It is shown that vacancies and impurities in the position of metal atoms may drastically change the band gap, even leading to appearance of the metallic properties, whereas substitution of chalcogen atoms by isovalent atoms changes the properties not so sharply. The ways of possible applications of heterostuctures with tunable band gaps for creation of transistors, light-emitting diodes, photoelectrochemical cells, photovoltaic and optoelectronic devices are proposed and the advantages of such devices in comparison with commonly used analogues are discussed.

A study on the electronic properties of Graphene Nanoribbons using the Offset Logarithm function

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[5] Centre for Advanced Materials Research, Sharjah, United Arab Emirates
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[7] Department of Physics and Astronomy, University of Western Ontario (UWO), London, ON, Canada

Graphene Nanoribbons (GN), being an important class of next-generation carbon materials, are of immense interest in the field of material science. They find their applications in electronic and opto-electronic devices, transparent conducive films, sensors and more. The investigation of electronic properties of graphene is key to unlocking its potential applications in many scientific domains. A variation of the generalized Lambert W function, called the Offset Logarithm function has been found to have important applications in different fields such as physics, engineering, mathematical biology, and more. An example of this is the work of Castro Neto *et al.* This work is concerned with the study of the electronic properties of zigzag GN. In the present work, we use the generalized Lambert W function and its properties to study the eigenvalue equation of the massless Dirac equation applied to the study of zigzag GN. Solutions to this equation are exclusively real or pure imaginary. There is an infinite number of pure complex solutions. They are computed numerically for different nanoribbon widths and verified using the analytically obtained bounds. Furthermore, we are studying the effects of the nanoribbon width and determining the parameters that significantly affect the solutions. Other 2D materials can also be studied using the present approach.
Keywords: Graphene nanoribbons, Generalized Lambert W function, 2D materials, Dirac equation.

Soft, flexible and transparent graphene-based active spinal cord implants for optogenetic studies

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Patients affected by spinal cord injuries (SCI) are usually unable to perform trivial motor activities and thus, for therapeutic purposes, epidural spinal cord stimulation (ESCS) is currently used. Moreover, more exploratory research, using optogenetics, is being conducted in rodents for a better understanding of the mechanisms that occur while delivering specific therapies. However, the availability of tailored neurotechnologies for such experiments is limited.

This work reports the development and characterization of flexible, active spinal cord implants with optogenetic compatibility[1,2] (Fig.1). A scalable and reproducible microfabrication process has been developed, using graphene[3], a transparent, flexible and conductive material, to form the electrodes and interconnects of the implant. Small and thin[4] electronic chips were assembled via flip-chip bonding processes either on graphene or on metal-on-graphene layers. Soft, polymeric encapsulation was employed to sustain the high flexibility and transparency of the implant. The result is an active prototype consisting of a multi-layered graphene structure between two polymeric-based encapsulation layers, with thin chips integrated on the implant and test pads for interconnection to the outside world.

Raman spectroscopy and optical transmittance were employed for the characterization of the graphene layer while cyclic voltammetry and electrochemical impedance spectroscopy were performed to benchmark the electrical properties of the device. The assembly process of the chips was evaluated using four-point electrical measurements.

In this work, the first transparent, graphene-based active implants have been developed (Fig. 2 and Fig. 3). The prototypes were extensively characterized and the results showed a transparency of ~80 % as well as no deterioration over time when soaked in saline solution or when bent under various angles. The graphene electrodes showed an impedance of ~8 kΩ at 1 kHz frequencies and the resistance after the bonding process ranged from 10 mΩ up to 16 Ω for individual connections, depending on the substrate used.

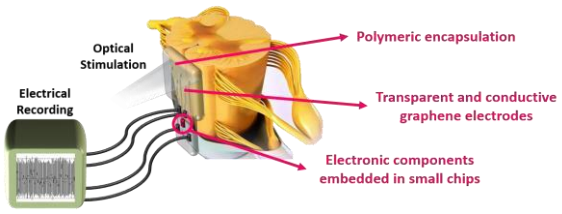

Fig. 1. Envisioned structure of the proposed system

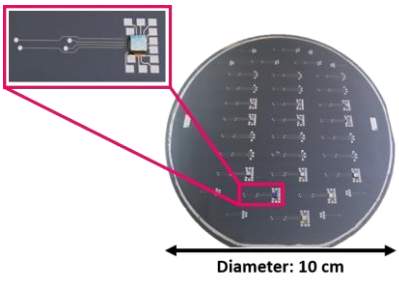

Fig. 2. Active prototypes developed on a silicon wafer

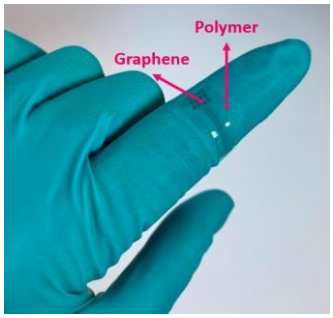

Fig. 3. Soft, flexible, graphene-based implants

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4. V. Giagka, N. Saeidi, A. Demosthenous, and N. Donaldson, "Controlled silicon IC thinning on individual die level for active implant integration using a purely mechanical process," in Proc. *ECTC 2014*, Orlando, FL, USA, May 2014, pp. 2213 – 2219.

WS3	
16:30-16:45	**INVITED (V)**
16:45-17:00	**Dr. Mark Birch, University of Cambridge, UK** Using nanoscale interactions to influence the repair and regeneration of osteochondral injuries
17:00-17:15	**INVITED**
17:15-17:30	**M. Stojanovic, Columbia University Irving Medical Center, USA** Molecular Computing on Cell Surfaces
17:30-17:45	**E. Vasileiou Nanotechnology Lab LTFN, AUTh, Greece**
17:45-18:00	Development of a titanium nitride nanoparticles-based lateral flow assay for acute lymphoblastic leukemia diagnosis

Using nanoscale interactions to influence the repair and regeneration of osteochondral injuries

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Musculoskeletal disease significantly impacts on the day-to-day living and wellbeing of many patients. Osteoarthritis (OA), the loss of cartilage and associated bone and soft tissue changes forms a major part of this issue. Providing therapeutic approaches that address early OA and prevent or reduce the likelihood of total joint replacement is a focus for many research teams. Current surgical approaches include microfracture and autologous chondrocyte implantation and whilst new cartilage tissue is formed, these procedures don't reproduce the original hyaline cartilage. Our studies seek to understand how therapeutics and/or cells can be delivered into the synovial joint to better influence the repair and regeneration of the damaged tissue and so alleviate pain and restore function. A number of different cell types have coordinated roles in the process of repair, including stromal cells such as mesenchymal stem cells (MSCs) and cells from the haematopoietic lineages including monocytes and natural killer cells. The spatial and temporal nature of tissue repair led us to consider how the context of these cell interactions could influence their cross talk and we have used a number of different 3D cell environments, ranging from fibrin and collagen to protein engineered and chemical polymers to investigate how cell-matrix interactions influence the immunomodulatory activity of MSCs. To address the mechanistic basis for differential cell response we have manipulated these environments at the nanoscale and evaluated the implications of altering parameters of matrix stiffness, cell adhesion ligand and growth factor display on cell function. Our ongoing work aims to exploit the manipulation of the tissue repair environment to influence processes, including chondrogenesis and vasculogenesis.

Molecular Computing on Cell Surfaces

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We will present a self-assembly process on surfaces of cells that will execute molecular computing cascades, and if all conditions (presence or absence of cell surface markers) are satisfied, this process will label very narrow subpopulation of cells. This protocol for cell isolation based on this self-assembly is able to condense multistep procedures that are typically used to isolate the very same narrow subpopulations into a single step, one-pot procedures. The advantage of this rapid, single step process is that it minimizes damage to cells and preserves their health, thus being suitable for clinical cell-based therapies in which health of cells is paramount. We will describe optimization of individual components, antibody-oligonucleotide conjugates, as well as conditions that were used to isolate grafts of cells that were subsequently tested in humanized mice disease models, with results at superior to gold standard protocols.

Friday 10th July

WS2

	WS2 Timber Hall 2 & Virtual Room NN (Group A) **Chair: S. Kassavetis, Nanotechnology Lab LTFN**
11:00-11:15	**A. Wosztyl, University of Warsaw, Poland (V)** A gigantic Faraday effect in a semiconductive polymer doped with Fe2O3 nanoparticles
11:15-11:30	**M. Zuena Università degli Studi "Roma Tre", Italy (V)** An innovative multifunctional TEOS-based coating with antifouling properties for stone materials: comparison between commercial biocide and natural antifoulant product
11:30-11:45	**A. Kaldeli-Kerou PLiN Nanotechnology SA, Greece** Copper-based Nanoparticles for Agricultural Applications
11:45-12:00	**P. Kutálek, University of Pardubice, CZ (V)** Ablation of binary chalcogenide glasses by UV ns laser
12:00-12:15	**Maria Stefanidou, AUTH** Nanoparticles controlling self-healing properties in cement pastes
12:15-12:30	**S. Pashayan, The Institute for Physical Research of NAS of Armenia, Armenia (V)** Copper Oxide-based Thin Films and Heterostructures: Fabrication and Properties Investigation
12:30-12:45	**INVITED (V)**
12:45-13:00	**Vasileios Koutsos, The University of Edinburgh, United Kingdom** Microbubble Agents for Biomedical Applications: Focus on NanoMechanics and the NanoShell

A gigantic Faraday effect in a semiconductive polymer doped with Fe_2O_3 nanoparticles

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The Faraday effect – the rotation of polarization plane of light passing through a medium in external magnetic field – in materials which do not contain magnetic ions, is a weak phenomenon: detection of Faraday rotation requires either long optical path or very strong magnetic fields. In order to enhance so called Verdet constant – the proportionality parameter between the angle of rotation and magnetic field – one can consider doping a material with magnetic ions. This approach was quite successfully tested in various glasses. One of the potential alternatives of transparent materials are organic polymers, which have not been extensively tested in this regard. This group of materials poses potential properties such as saturating in much larger magnetic fields, low sensitivity to temperature changes, flexibility and ease of manufacture. The most problematic aspect of these materials is relatively small values of Verdet constant in regions far from optical resonances. The goal of this project is to obtain hybrid organic-inorganic materials with higher values of Verdet constant. It has been concluded that semiconductive polymer poly-3-hexylthiophene (P3HT) doped with iron (III) oxide nanoparticles is a promising candidate. Hybrid materials have been characterized by UV-Vis spectroscopy. The Faraday effect was measured with a magnetic coil (0.4 T) for different wavelengths (450 nm, 543 nm, 594 nm, 604 nm, 612 nm, 633 nm, 640 nm). It was observed that for iron oxide-doped samples with a wavelength greater than 594 nm reveal higher values of the Verdet constant.

Copper-based Nanoparticles for Agricultural Applications

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The growing environmental requirements and related European legislation regarding the use of plant protection products (biocides, herbicides, pesticides, insecticides, etc.), pose serious risks to the competitiveness of domestic agricultural production, as pests and insects are becoming increasingly resistant to conventional plant protection products. Copper and its compounds are widely used in agriculture due to their antibacterial and antifungal activity against various plant pathogens.

The aim of this research is the development of copper oxide/hydroxide nanoparticles, through a wet chemical reduction process, that provide enhanced protection for a specific category of crops. During the procedure, several parameters were evaluated, such as different reagents (e.g., copper salts and stabilizing agents), pH, temperature, concentrations etc. The final products were characterized with respect to average size, size distribution (Dynamic Light Scattering, DLS), zeta-potential (Laser Doppler Electrophoresis, LDE), characteristic peak at specific wavelength (Ultraviolet-Visible spectroscopy, UV-Vis), functional groups (Attenuated Total Reflectance, ATR), and morphology (Transmission Electron Microscopy, TEM). Copper-based nanoparticles were found to be monodispersed with an average diameter in the range of 5-15nm and a spherical morphology.

Ablation of binary chalcogenide glasses by UV ns laser

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This study is focused on the interaction of binary (As_2S_3, As_2Se_3, GeS_2 $GeSe_2$ and $GeSe_3$) chalcogenide bulk glasses and thin films with the UV nanosecond pulsed laser. This leads to the reproducible craters formation and also due to the suitable material behavior, the craters can be used as microlenses. The craters topography created in bulk glasses or thin films by the digital holographic microscopy (DHM) was mainly studied and verified by atomic force microscopy (AFM). Phase imaging AFM mode shows the negligible mechanical properties changes during the craters formation. The chemical composition by EDX analysis was checked and it reveals the partial oxidation for the sulfur-based glasses. The influence of pulses number and intensity of pulses on the craters formation was studied. The most convenient for usage from the point of ablation rate (ablated matter volume per pulse) is As_2S_3 glass (620 μm^3/pulse) as it has the lowest melting temperature and density in comparison with other studied glasses. On the other hand, the laser induced ablation threshold (LIAT) that expresses how much energy is material able to absorb without any damage, is the lowest for GeS_2 glass (0.05 J/cm^2) as it has the largest photons penetration depth and lowest value of thermal diffusivity among others. Finally, the sets of gratings in the form of craters and lines by laser direct writing were created and their functionality for the diffraction of visible light radiation was checked.

Nanoparticles controlling self-healing properties in cement pastes

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Despite their many advantages, cement-based materials remain vulnerable to cracking due to interaction of different causes (ambient conditions, heat-humidity changes, shrinkage, oxidation of reinforcement, etc.). Cracks may limit the applicability of the materials but mainly they restrain their durability. Often, intervention and repair are required but they increase the construction cost. Towards this direction, in recent years, there has been an ongoing effort to develop advanced materials with increased lifespan through the ability of materials to self-heal their deficiencies (gaps) mainly when these flaws are first formed. A safe way to create conditions in order to be able to synthesize products that will heal gaps, is the nano-sized admixtures inserted into the material.
The present study combines the use of nanoparticles for the control of cement paste healing phenomena. The aim is to combine nanosilica (nS) and nano-lime (nL) to achieve a cohesive structure with small cracks (the main role of nS) that will heal in the presence of calcite (the main role of nL) with simultaneous additional CSH compounds formation. Controlled fracture was created in the compositions prepared (pre-cracking), using the 3-point bending technique. The specimens were cured under water and at the age of 28 days the mechanical, physical and microstructure properties were recorded for the reference composition and the compositions with nano particles. The results indicate enhanced strength especially in the presence of nS, reduced porosity and capillary absorption, especially in the presence of nL. Additionally, significant crack width reduction is recorded in nanomodified compositions. Smart materials that can heal their flaws due to the presence of small number of nanoparticles is a promising advantage in the construction sector.

Copper Oxide-based Thin Films and Heterostructures: Fabrication and Properties Investigation

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Fabrication of copper oxide nanoscale thin films is of both fundamental and practical interest for their use in the production of solar cells, sensors, photodetectors, and other optoelectronic devices. In the present work the structural, morphological, optical and i-V characterization of copper oxide-based thin films and heterostructures synthesized by magnetron sputtering technique are discussed. The prepared ZnO and CuO thin films with thickness of 100 nm and 200 nm respectively and an average grain size below 50 nm have nearly uniform surface structure. To fabricate n-ZnO/ p-CuO structure these films were deposited onto the Indium Tin Oxide (ITO) coated glass substrates and followed by the annealing at 270°C. Silver paste was used as the top contact. To determine the characteristics of the films obtained and ITO/ZnO/CuO/Ag heterostructures SEM, EDX, AFM, surface roughness measurements, UV–Visible absorption and Raman spectroscopy used. The studies of the optical properties of bilayer structure showed an increase in absorption in the region above 400 nm corresponding to the Cu2O phase and absorption band at 600–700 nm attributable to CuO. These results are in good agreement with the results of Raman analysis.
The direct and indirect band gaps were calculated using Tauc plot and estimated to be 3.0 eV and 1.4 eV, These results are corresponding well to Eg value interval for Cu2O and CuO thin films, respectively. The band gap for the obtained zinc oxide thin films was around ~ 3.3 eV, that is slightly lower than the value for the bulk material (Eg = 3.37 eV). The current-voltage characteristics of the ITO/n-ZnO/p-CuO/Ag structure were studied at room temperature under dark and illuminated conditions. The increase in current was observed under the illumination, while the direct and reverse switching indicates a photosensitive structure.

Microbubble Agents for Biomedical Applications: Focus on NanoMechanics and the NanoShell

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Stable, haemodynamically inert, hollow, micrometre-size spheres, composed of a shell (usually phospholipid-based) which encapsulates an inert gas are used as ultrasound contrast agents and are normally referred to as microbubbles (MBs). They are smaller than the smallest blood vessel of a human body to allow improved visualization of the vascular bed and differentiate vascular patterns of tumours non-invasively. Such nano-shelled microstructures can be used as carriers for drug/gene delivery, which is a topic of much current interest in biomedical research. Furthermore, with appropriate surface modification such MBs can acquire targeting capability for certain cell types (e.g. cancerous cells). Their nanomechanical properties are extremely important since they have to be stable for considerable time until they rupture/degrade under specific conditions in order to release their load in the right place and at the right time. Moreover, materials at the nanoscale (such as thin-shell structures) may behave differently to those on the macroscale, so predicting their mechanical properties presents a challenge. We have conducted a systematic study of phospholipid-shelled MBs in their natural hydrated state employing tapping-mode atomic force microscopy (AFM), state-of-the-art quantitative imaging (QI)-mode AFM, and focused-ion-beam (FIB) cryo-scanning electron microscopy (cryo-SEM). Combining these techniques, we show unequivocally and for the first time that the thin phospholipid shell of the MBs is ca. 6.5 nm and corresponds to a trilayer. We discuss in detail the structure of the shell, including the polyethylene glycol (PEG) layer which surrounds the phospholipid shell. Furthermore, using the measured value of the shell thickness we revisit the MB nanomechanics (based on AFM force-distance curves) showing which mechanical theories predict more accurately their mechanical properties.

WS3	
	Timber Hall 2 & Virtual Room NN (Group A) **Chair: C. Gravalidis, Nanotechnology Lab LTFN**
14:00-14:15 14:15-14:30	**INVITED (V)** **Prof. Ioannis S. Vizirianakis, Department of Pharmaceutical Sciences, AUTH, Greece** Implementation of pharmacogenomics knowledge in the clinical setting to guide precision cancer therapy decisions
14:30-14:45 14:45-15:00	**INVITED (L)** **Dr ilise L Feitshans JD and ScM and DIR** Safernano by design: enhancing commercialization of nano-enabled products
15:00-15:15	**A. Ihnatsyeu-Kachan Korea Institute of Science and Technology, Republic of Korea (V)** Biomimetic Gene-Silencing Nanoplatform for Therapy of Liver Cancer
15:15-15:30	**M. Kiseleva Université Laval, Canada (V)** A 3D-printed hybrid hydrogel-nanoparticle formulation as a localized delivery system for cervical cancer therapy
15:30-15:45 15:45-16:00	**KEYNOTE (V)** **Prof. Roger Leblanc** Carbon Dots as Novel Vehicle for Drug Delivery in Modern Medical Healthcare
16:00-16:30	**KEYNOTE** **S.. Vainio, Oulu Central Hospital Oulu University, Oulu, Oulu, Finland** Skin as an organ in homeostasis and disease biomonitoring

Implementation of pharmacogenomics knowledge in the clinical setting to guide precision cancer therapy decisions

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Somatic mutations acquired by tumor cells accompanied with alterations in RNA and protein levels, posttranscriptional and post-translational modifications, and epigenomic deregulation, constitute the ground where cancer cells exhibit hallmarks with the capacity of unlimited proliferation rate and blockade of differentiation, apoptosis and autophagy processes. Moreover, research and clinical efforts focusing on delivering improved safety and efficacy profiles of cancer therapeutics are hindered by tumor cell heterogeneity and spatial microenvironment diversity within the malignant tissue. Consequently, real-time situations in the clinical setting exist in which the oncologist asks for knowledge-guided solutions upon confronting the therapeutic failures related to the tumor cell heterogeneity. To some extend such heterogeneity refers to the mutational status, epigenetic phenomena, cell interactions within the tumor microenvironment. To this end, innovative tumor profiling methodologies are utilized to elucidate the pharmacogenomic landscape of tumor cells in order to support the molecularly-guided delivery of therapeutics. However, there is still limited utilization of the technology especially in small private oncology practices. Thus, our effort has been to assess how molecularlyguided interventions, within the concept of precision medicine strategies, improve disease response rates in small and medium size oncology centers. The finding of clinically-actionable relationships between tumor biomarkers and drug responses through the application of pharmacogenomics-based molecular profiling has been applied to primary tumor patient samples. Notably, improved clinical outcomes are achieved by providing the physicians with expert-guided, standardized and easily interpretable knowledge, by translating molecular profiling data to support clinical decision-making. In our case, pharmacogenomics driven recommendations favorably impacted cancer therapy progression upon proper implementation in the routine private oncology practice, a fact that will be analyzed and discussed. Relevant reference

Astras G., Papagiannopoulos CI, Kyritsis KA, Markitani C, Vizirianakis IS. (2020). Pharmacogenomic testing to guide personalized cancer medicine decisions in private oncology practice: A case study. Front. Oncol.

Safernano by design: enhancing commercialization of nano-enabled products

Dr ilise L Feitshans JD and ScM and DIR

This presentation provides an overview of emerging nanoregulations; a treacherous swamp of new laws draft laws and pre-existing laws. Additionally there are rules emerging from powerful opinion leaders who have expertise but not regulatory authority, such as some USA federal government agencies and the World Health Organization (WHO). This overview of the emerging law explores USA OSHA and EU REACh .and NIOSH RELs (Recommended Exposure Limits) for carbon nanotubes and nanofibers, TiO2 and best practices for nanomaterials used by both workers and consumers despite the unquantified risks posed by nanomaterials, and also reviews laws about environmental health during the life cycle that includes disposal and waste. The proliferation of these rules means that researchers and their employers must have a safety and health compliance program for nanomaterials. This presentation describes the recommended procedures. The existence of WHO guidelines for workplace exposure to nanomaterials and several unprecedented applications of precautionary principles suggests that regulations are here to stay, even though no data yet exists demonstrating a link between exposure and proven harm. This presentation offers practical steps for due diligence and compliance with these rules.

Biomimetic Gene-Silencing Nanoplatform for Therapy of Liver Cancer

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RNA interference (RNAi) is a natural process of post-transcriptional gene regulation. Short double-stranded RNA molecules, small interfering RNAs (siRNAs), carry out the process of RNAi. Using synthetic siRNAs, we can stop the production of an undesirable protein related to a disease even before it is synthesized inside the cell. FDA approved the first gene-silencing therapy employing RNAi – patisiran – in August 2018.

The goal of this study is to develop a biomimetic gene-silencing nanoplatform based on reconstituted high-density lipoprotein nanoparticles (HDL-NPs) and siRNAs to ensure a better quality of life of patients with liver cancer. For this, we selected novel therapeutic targets in hepatocellular carcinoma and incorporated siRNA against these targets into HDL-NPs. We modulated the composition of HDL-NPS to achieve the highest encapsulation of siRNA, and are in the process of comprehensive efficiency assessment of the nanoplatform using liver cancer cell lines (cellular uptake, cell viability assays, gene silencing efficiency). Further, we plan to perform the optimization of the nanoplatform for high accumulation in liver cancer using an in vivo tumor xenograft model.

The liver is a major organ of cholesterol metabolism, and therefore hepatocytes express many receptors for HDL. Via the SR-BI receptor, HDL-NPs are capable of precise liver targeting and release of the medication directly into the cytosol, where the process of protein synthesis happens. This approach harnesses the natural mechanism of lipid transport and can be employed to achieve positive therapeutic outcomes in liver disease using gene-based drugs.

A 3D-printed hybrid hydrogel-nanoparticle formulation as a localized delivery system for cervical cancer therapy

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The localized delivery plays an important role in the therapy of cervical cancer. The development of the personalized dosage forms is essential for increasing patient compliance and could be achieved using 3D-printing technology. In this study, a localized delivery system composed of ultra-small gold nanoparticles (AuNPs) and a 3D-printed Pluronic F127-alginate hydrogel was prepared. The applicability of a 3D-printed hybrid formulation for intravaginal delivery was demonstrated by studying the following parameters: 1) printability of a hydrogel ink; 2) hydrogel degradation and AuNPs release; 3) cytocompatibility. The printability of the prepared hydrogel ink was evaluated by the fabrication of the scaffolds in a lens-shape (Ø 10mm) and a smaller tube-shape (Ø 3mm). *In vitro* degradation of the gels and release of AuNPs were investigated in simulated vaginal fluid and monitored using SEM, FTIR, and micro-XRF imaging. As a result, the 3D-printed gels were fabricated with high resolution down to 0.2 mm and excellent reproducibility (n>50). FTIR analysis demonstrated that the degradation of the gels was governed by the dissolution of the Pluronic F127 component out of the polymer network. SEM revealed the increase in pore size by 11 times by the end of degradation. Around 80% of encapsulated AuNPs were released during the first two days of incubation. The complete release was achieved after the fifth day and confirmed by micro-XRF analysis by the absence of the characteristic Au lines (Lα 9.713 keV and Mα 2.123 keV) in the spectrum of the degraded gel. Finally, the Pluronic F127-alginate formulation exhibited no detectable cytotoxicity in HeLa and BT-474 cells.

Carbon Dots as Novel Vehicle for Drug Delivery in Modern Medical Healthcare

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Carbon dots (CDs) have triggered great attention due to their unique properties such as small size (1-10 nm), excellent photoluminescence (PL), high water-dispersity, biocompatibility, nontoxicity and abundant surface functionalities. They have been widely explored for applications in catalysis, bioimaging, sensing, drug delivery, and nanomedicine. In this presentation, I will introduce diverse preparations and characterizations of CDs. These CDs were prepared from either "top-down" or "bottom-up" strategies and rigorously characterized by spectroscopies and microscopies. I will also exhibit various applications of the CDs developed in our lab. (1), a major medical challenge one faces to treat central nervous system (CNS) related diseases is to cross the blood-brain barrier (BBB). Recently, in vivo experimental observations suggested that plenty of CDs developed in our group could cross the BBB to enter the CNS of zebrafish with different mechanisms; (2), thanks to the abundant carboxyl groups on the surface, CDs prepared with carbon nanopowder could be conjugated with transferrin and two anticancer drugs to construct a triple-conjugated drug delivery system. The system showed a synergistic effect on the treatment of glioblastoma brain tumor; (3), our study has shown that CDs prepared with carbon nanopowder bind to calcified bone structures of live zebrafish larvae with high affinity and selectively. Furthermore, we have observed this property is unique to the CDs developed from carbon nanopowder and other CDs preparations did not show any interaction with the bone; (4), CDs have constantly shown the capability to inhibit beta-amyloid (Aβ) secretion and fibrillation, which exhibits a great potential of CDs as an effective nanomedicine and drug nanocarrier to treat Alzheimer's disease (AD); (5), a pilot study showed a versatile nanocarrier could be assembled via conjugation between distinct CDs to fulfil multitasks.

Novel Avenues to Biomonitoring Changes in Homeostasis and Disease

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Non- or minimally invasive capacity to conduct biomonitoring of human physiology and disease would advance greatly the aims to develop the preventive and personalized medicine measures. In our research line we approach this by developing integrated technological applications. For example, being on the surface of the body, the skin may provide novel means to identify disease related biomarkers such as changes in blood glucose level. Our recent evidence is starting to suggest that the nano- and micro size secreted extracellular vesicles (EVs, 30-1000 nm) serve as the tools to diagnose changes in homeostasis and disease. Thus, the EVs may offer means to develop novel biosensor assembly strategies including the skin.

In addition to the EVs we are taking use of gene edited, programmed stem cells and organoids derived from them in diagnostics development taking use of the Finnish biobanks and cohorts. Data will be presented that the skin as an organ serves as a useful organ that reflects the changes in homeostasis. Proteomic screen conducted in the skin in the skin via experimental *in vivo* mouse model of type I diabetes and controls identified Trisk95 as an essential factor whose expression is induced in the skin independently of insulin action in correlation with changes in intracellular calcium. Together, the data consistent with the conclusion that the skin reacts to systemic changes such as blood glucose and that the Trisk95 channelling model is a promising biomarker for a glucose biomonitoring technology assembly.

WS3

	Timber Hall 2 & Virtual Room NN (Group A) **Chair: C. Gravalidis, Nanotechnology Lab LTFN**
16:30-16:45	**KEYNOTE (V)**
16:45-17:00	**Prof. Elisa Konofagou, Columbia University, USA** Noninvasive Drug Delivery Through the Opened Blood-Brain Barrier for the Treatment of Brain Diseases - From Mice to Humans
17:00-17:15	**INVITED (V)**
17:15-17:30	**C. Kiparissides Centre for Research and Technology Hellas, Greece** Recent Developments in Antigen-Specific Immunotherapies for the Treatment of Multiple Sclerosis
17:30-17:45	**C. Kiparissides Centre for Research and Technology Hellas, Greece (V)** SNEDDS Incorporating two Adjuvants as Potential Nanocarriers for Vaccines
17:45-18:00	**EU PROJECT (V)** **D. Schmid; Swiss Center for Electronics and Microtechnology (CSEM), Switzerland** Low-cost, versatile colorimetric reader for reactivity assessment of nanomaterials
18:00-18:15	**S. Petanidis, Aristotle University of Thessaloniki, Greece.** Dual photothermal MDSCs-targeted immunotherapy inhibits lung immunosuppressive metastasis by enhancing T-cell recruitment.
18:15-18:30	**F. Meier Postnova Analytics GmbH, Germany (V)** Multidetector Field-Flow Fractionation Techniques for the Characterization of Liposomal Drug Formulations
18:30-18:45	**M. Natalia D.S. Cordeiro, University of Porto, Portugal** In Silico Tool For Probing The Multiple Antibacterial Profiles Of Nanoparticles By A Qsar Perturbation Model
18:45-19:00	**E. Ismail, Cape peninsula university of technology, South Africa (V)** The green synthesis of Nobel metals nanoparticles via medicinal plants extracts and their biological activity against Streptococcus mutans bacterial strain

Noninvasive Drug Delivery Through the Opened Blood-Brain Barrier for the Treatment of Brain Diseases - From Mice to Humans

Elisa E. Konofagou[1,2], Maria Eleni Karakatsani[1], Antonios Pouliopoulos[1], Shutao Wang[1], Robin Ji[1], Shih-Ying Wu[1], Mark Burgess[1] and Hermes Kamimura[1]

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The blood-brain barrier (BBB) poses a formidable impediment to the treatment of adult-onset neurodegenerative disorders preventing most drugs from gaining access to the brain parenchyma. Focused ultrasound (FUS), in conjunction with systemically administered microbubbles, has been shown to open the BBB locally, reversibly and non-invasively. In this study, application of FUS at the early stages of neurodegenerative disease, such as Alzheimer's and Parkinson's in conjunction with neurotrophic drug (protein or gene) delivery will be presented in terms of neuroprotection and neurorestoration of the dopaminergic pathway in a PD animal model. The objective is to induce localized drug delivery in the brain, such as the hippocampus and the substantia nigra, by taking advantage of the type of interaction between ultrasound waves and microbubbles. The result is the reversible opening of the blood-brain barrier in the brain capillaries; allowing thus the transport of molecules that would help image and/or treat the afflicted brain regions. Over these past 15 years, ourr group has demonstrated feasibility of FUS was capable of generate highly focused and transient BBB openings in mouse and non-human primate (NHP) brains through intact skull and skin in vivo; therefore, completely noninvasively. We have also identified the mechanism by which the BBB opens involving transcellular diffusion at low FUS pressures and tight-junction disruption at higher pressures. By optimizing this novel drug delivery system such as neurotrophic factors for effective neuronal restoration in deep-seated brain regions such as the substantia nigra as well as inducing an immune response for reduction of the amyloid plaque and tau load in the hippocampus and the substantia nigra. The final part of the presentation will entail translation to clinical application in the treatment of early Alzheimer's.

Recent Developments in Antigen-Specific Immunotherapies for the Treatment of Multiple Sclerosis

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Multiple sclerosis (MS) is an autoimmune disease of the central nervous system and is considered to be the leading non-traumatic cause of neurological disability in young adults. Current treatments for MS comprise long term immunosuppressant drugs and disease-modifying therapies (DMTs) designed to alter its progress with the enhanced risk of severe side effects. The Holy Grail for the treatment of MS is to specifically suppress the disease while at the same time allow the immune system to be functionally active against infectious diseases and malignancy. This could be achieved via the development of immunotherapies designed to specifically suppress immune responses to self-antigens (e.g., myelin antigens). The present study is attempting to highlight the various antigen-specific immunotherapies developed so far for the treatment of multiple sclerosis (e.g., vaccination with myelin derived peptides/proteins, plasmid DNA encoding myelin epitopes, tolerogenic dendritic cells pulsed with encephalitogenic epitopes of myelin proteins, attenuated autologous T cells specific for myelin antigens, T cell receptor peptides, carriers loaded/conjugated with myelin immunodominant peptides, etc) with respect to their in vivo and clinical evaluation outcome and the challenges they face in order to be translated from animal models to patients. It also seeks to unravel the mechanisms involved in the immunopathogenesis of the relapsing remitting and progressive MS as well as the mechanisms of action of the developed tolerance-inducing vaccines.

SNEDDS Incorporating two Adjuvants as Potential Nanocarriers for Vaccines

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Self-nanoemulsifying drug delivery systems (SNEDDS) are isotropic mixtures of oil, surfactant and cosurfactant spontaneously forming an o/w nanoemulsion upon mixing with water. The formed nanoemulsion is a thermodynamically stable system with extremely small droplet size (i.e., 50 nm). SNEDDS are typically used to enhance the oral bioavailability of poorly water soluble drugs and there already exist marketed formulations of hydrophobic drugs based on SNEDDS technology. Recently, the administration of hydrophilic drugs including therapeutic peptides has been also demonstrated. The present study deals with the development of a novel SNEDDS formulation for vaccine delivery containing two different adjuvants (e.g., squalene and tocopherol-α). Various excipient combinations, and weight ratios of adjuvants, surfactant and cosurfactant for each combination were evaluated with the aid of ternary phase diagrams. The selected formulation was characterized by an average droplet diameter of 28 nm and adjuvant concentrations equal to 250 μg squalene and 100 μg tocopherol-α per 100 μl dose. In order to increase the adjuvants' concentration in the formulation, the effect of the volume of the aqueous phase on the droplet diameter was examined. It was shown that a substantial decrease in the volume of the aqueous phase (e.g., from 99 mL down to 4 mL) resulted in a nanoemulsion with an average droplet diameter of 40 nm and adjuvant concentrations equal to 5000 μg squalene (≥ of squalene concentration in ADAVAX) and 2000 μg tocopherol-α per 100 μl dose. Furthermore, the nanoemuslion was shown to exhibit storage stability at 4^{o}C for more than 4 weeks. The developed SNEDDS formulation could thus be considered as a promising strategy for the delivery of vaccines.

Low-cost, versatile colorimetric reader for reactivity assessment of nanomaterials

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Engineered nanomaterials are being produced in exponentially increasing quantities, due to their unique physical and chemical properties and the improved performance of final products, and therefore spur technological and economic progress. A comprehensive risk assessment of these new materials is crucial to create new adequate regulations. One key parameter is the reactivity of nanomaterials, for which there is a substantial lack of techniques for reproducible assessment. In the frame of the European project ACEnano, CSEM developed a low-cost automated solution for reactivity monitoring of nanomaterials – a risk assessment tool that can be used to reveal correlations associated with health and environmental impacts. The presence of nanoparticles is detected by a relatively simple catalytic reactivity assay with a colorimetric detection in complex samples.

Here we present a novel simple and affordable optoelectronic system for monitoring of 24 samples in parallel. Our approach uses differential two-wavelengths monitoring to measure static and dynamic changes in absorbance, which allows to quickly screen for the presence and reactivity of nanoparticles in samples. We could show that, unlike current analytical methods, our solution does not require highly trained personnel, nor expensive instrumentation and time-consuming sample preparation, is easily transportable and can be used for tests in the field. The system has been validated and reproducibility has been shown in comparison to a manual cuvette-based method.

Dual photothermal MDSCs-targeted immunotherapy inhibits lung immunosuppressive metastasis by enhancing T-cell recruitment.

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Immunosuppressive chemoresistance is a major barrier in lung cancer treatment. In this study, we introduce a model of precise immunosuppressive-based nanotherapy by designing and delivering biocompatible MDSC-targeted nanocarriers (NCs) into the lung tumor microenvironment. This is accomplished by conjugating L-Norvaline and Sunitinib integrated into biodegradable nanosomes in order to facilitate inhibition of tumor-supporting immunosuppression. Findings show that treatment with NCs increased apoptosis and significantly reduced tumor volume and Ki-67 antigen expression respectively. Biodistribution analysis revealed an increase in drug circulation time, as well as a greater accumulation in lung and peripheral tissues. In addition, these nanospheres showed increased PTT efficiency and tumour targeting ability as evidenced by highly efficient tumour ablation under near infrared (NIR) exposure. Significant tumor reduction was observed due to recruitment of cytotoxic T-lymphocytes. Taken together, our findings provide a novel nanodrug delivery strategy for the inhibition of MDSC-related immunosuppression. in lung tumor microenvironment and provide a new approach for the efficient treatment of metastatic lung cancer.subsets were characterized by the reduction of Gr/CD11b cell population in blood and tissue samples. In addition, these nanospheres, showed increased PTT efficiency and tumour targeting ability as evidenced by highly efficient tumour ablation under near infrared (NIR) exposure. Significant tumor reduction was observed due to recruitment of cytotoxic T-lymphocytes, followed by downregulation of immunosuppressive Foxp3^{+} Treg cells. Taken together, our findings provide a novel nanodrug delivery strategy for the inhibition of MDSC-related immunosuppression in lung tumor microenvironment and provide a new approach for the efficient treatment of metastatic lung cancer.

Multidetector Field-Flow Fractionation Techniques for the Characterization of Liposomal Drug Formulations

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Field-Flow Fractionation (FFF) belongs to the flow-based separation techniques, where separation of dissolved, suspended and dispersed sample constituents in the size range of 1 nm to approx. 50 µm is achieved within a thin, ribbon-like channel without stationary phase. In FFF separation of different sample constituents is induced by a force field that acts perpendicular to the channel flow, which transports the sample toward the channel outlet and further to the respective detectors. Depending on the applied force field, FFF can be divided into different subtechniques. In Asymmetrical-Flow FFF (AF4), a second flow, called cross flow, enables separation according to hydrodynamic size. By superimposing the cross flow field with an electrical field, Electrical Asymmetrical-Flow FFF (EAF4) additionally enables the separation according to charge thus gaining access to electrophoretic mobility and Zeta potential of the sample. In Centrifugal FFF (CF3), a centrifugal force field induces separation according to the mass of a respective sample.

Two FFF application examples for the characterization of liposomes are presented here. In the first study, CF3 coupled with UV-detection and offline microscopy was used to quantify the amount of non-encapsulated drug in a liposomal drug formulation by separating the free drug from the filled liposomes.

In the second study, EAF4 coupled with UV-, Multi Angle Light Scattering and Dynamic Light Scattering detection was used to characterize Liposomal Doxorubicin HCl under physiological conditions.

Both studies clearly highlight the capabilities of FFF-techniques for the comprehensive physico-chemical characterization of liposomes as they give valuable insights into crucial properties such as drug loading efficiency,

The green synthesis of Nobel metals nanoparticles via medicinal plants extracts and their biological activity against Streptococcus mutans bacterial strain

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A broad variety of different physical and chemical synthesis methods are existence for the synthesis of nanoparticles (NPs). Green synthesis approach is recently attracted more attention for the biogenic synthesis of metal NPs. This is for simplicity, eco-friendly, economically and mainly for medical and biological applications. In this study, different medicinal plants were selected to be evaluated for their potential activity in the synthesise of gold and silver nanoparticles. The screening of the different plant extracts was performed using 96 well plate method at 25 °C and 70 °C to study the effect of temperature on the NPs formation process. The NPs formation of was confirmed and characterized using UV- Vis, DLS, HR-TEM and EDX. The results reveal that, a well-defined NPs were obtained at high temperature (70 °C). HR- TEM images shows a formation of Gold NPs with an average diameter of 92 nm at 25 °C and 66 nm at 70 °C. The zeta potential values were observed to be negative and contributing to the stability of Au NPs. The HR-TEM also showed a polydispersity NPs which decreasing at higher temperature (70 °C). However, the results show that most of the silver nanoparticles synthesized at different concentrations of collected plant extracts are spherical. The stability of biosynthesized NPs in nutrient broth prior was conducted as well. Based on the results, selected plants extracts such as Pistacia atlantica, Rosmarinus officinalis, Junipers phoenicea and their biosynthesis NPs were tested against Streptococcus mutans bacterial strain. The results show slight differences in MIC values based on the plant extract used for the NPs formation. Also, the synthesised metallic NPs showed a promising bioactivity for developments of new antibacterial agents against S. mutans strains.

POSTER

WS1

P1-1 Study of Front Panel Electrode Coatings for Combined Visible and Short Wavelength Infrared Photodetectors
M. Aleksandrova Technical University of Sofia, Department of Microelectronics, Bulgaria

P1-2 Modeling the Optical Properties of Plasmonic Nanoparticles via Finite Element Analysis
Efstratios K. Antoniou, Aristotle University of Thessaloniki, Greece

P1-3 Plasmon sensitivity of different silver nanoplates obtained by “seed mediated growth”
M.Pulvirenti, University of Catania, Italy

P1-4 Fabrication of plasmonic transition metal nitride nanoparticles by ultrashort pulse laser ablation in liquids,
A. Koutsogianni, Nanotechnology Lab LTFN, Greece

Study of Front Panel Electrode Coatings for Combined Visible and Short Wavelength Infrared Photodetectors

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ZnO-Ga_2O_3 composite oxide films were RF sputtered and studied how the optical and electrical film properties are affected by the sputtering conditions and film thickness. The aim was to achieve low resistivity and at the same time, high transparency for the visible and near-infrared (NIR) electromagnetic range for the needs of simple, transparent and indium-free electrodes. A comparison was made with pristine ZnO and conventional indium tin oxide (ITO) films. We found that plasma power plays a crucial role in determining the optoelectronic properties of the deposited films for the fabrication of combined visible and short wavelength infrared photodetectors. RMS surface roughness of the ZnO-Ga_2O_3 films varied between 12.9 nm and 16.7 nm (for a film thickness of 250 nm) when plasma power density varied between 35 and 54 W/cm^2, respectively. The increase of the sputtering power narrowed the transmission band to the longer wavelength from the visible spectrum. The transparency in the NIR range varied between 83 and 96% and decreased with the plasma power increase, while the corresponding transparency in the visible range varied between 60 and 82%. The sheet resistance for the films under the best parameters conditions demonstrating the highest transmission in both electromagnetic ranges showed relatively low sheet resistance of 48 Ω/sq. The potential application of the prepared films is for VIS-IR detectors, used in robotics for spatial information gain, gaming and virtual reality and autonomous car navigation where day and night visions are equally important.

Modeling the Optical Properties of Plasmonic Nanoparticles via Finite Element Analysis

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Plasmon related optical properties of metallic nanoparticles can be valuable for a variety of applications in fields such as biosensing, biomedicine, electronics, energy harvesting, imaging and photocatalysis. Designing and optimizing nanoparticles is essential for the development of new innovative applications as well as for the evolution of existing ones. Numerical modeling simulations is a key tool for predicting and consequently controlling the optical response of plasmonic nanoparticles.

This study focuses on gold (Au) and silver (Ag) nanoparticles in water solution and especially on their extinction cross-section spectra. Geometries like nanorods, bipyramids, bicones and spheroids are being tested for different aspect ratios and sizes via computational simulations with the use of the 3D Finite Element Method (FEM). The calculations made in a wavelength range between 600 nm and 1300 nm, with a step of 5 nm. A spherical Perfectly Matched Layer (PML) was chosen for all the models and the mesh of nanoparticles was tetrahedral.

Our results show that the extinction cross-section from FEM analysis closely matches with the analytical solution in simple cases. Both have the same position of the extinction peak and full width half maximum (FWHM) of the spectra. We conducted simulations in a wide variety of geometries and aspect ratios for different sizes and it is also shown that the plasmons of the larger particles are redshifted and broadened in an obvious and measurable manner. In addition, for the geometry of the bipyramids, an effect of the shape of their base on plasmon resonance has been observed. In particular, pentagonal bipyramids have their resonances redshifted in relation to that of square bipyramids with the same aspect ratio.

Plasmon sensitivity of different silver nanoplates obtained by "seed mediated growth"

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Silver nanoparticles are potentially able to detect molecular specimen in solution because of their plasmon resonance features which can be tuned from near UV to near infrared. The plasmon sensitivity strongly depends on the nanoparticles' size and shape, so that a strict control in their fabrication is of crucial importance. For this reason, there exists a great ferment into the field of scientific research to obtain highly performant synthesis methods, also in sight of possible industrial applications.

In this work we present a study of the plasmon sensitivity for a variety of silver nanoplates prepared by a seed mediated growth method, having a wide range of plasmon resonances (from 400 to 1200 nm). Shapes and size have been carefully studied by SEM and AFM microscopies and a statistical survey of the particles' roundness has been considered. The sensitivity factors have been evaluated for different nanoplates, either in the colloidal state and after the deposition on suitable substrates, by performing extinction spectra after the interaction of the plates with different liquids, possessing a variety of refractive indices. We have found that silver nanoplates with plasmon resonances in the near infrared, give plasmon sensitivities greater by a factor of about 5 with respect to simple spherical clusters, either in the colloidal state or onto a substrate.

Fabrication of plasmonic transition metal nitride nanoparticles by ultrashort pulse laser ablation in liquids

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Plasmonic materials and devices have shown promising results both in electronic and biomedical applications Transition metal nitrides (TMNs) have emerged as an alternative to traditional plasmonic metals, such as gold and silver, regarding their plasmonic response in the biological window from 650 to 1350nm. [Patsalas et al., Mater. Sci. Eng. R Rep., 123, 1-55, (2018)]

In this work we synthesized transition metal nitride nanoparticles by pulsed laser ablation (PLA) using a picosecond and nanosecond Nd-YAG laser at wavelengths of 1064, 532, 355 and 266nm with the scope to use them as plasmonic materials in biological applications, such as biomedical sensing (e.g. Surface Enhanced Raman Spectroscopy-SERS). TiN coatings (thickness > 300 nm) were used as targets for the PLA process. In order to avoid oxidation of the produced NPs, the PLA process was made in liquid nitrogen medium followed by substitution with ethanol to eliminate the formation of unwanted byproducts.

The nanoparticles were characterized by Atomic Force Microscopy (AFM) and Transmission Optical Spectroscopy. We studied the dependence of the LSPR and the nanoparticles' geometry on the wavelength, the pulse duration, the laser fluence and the solvent. Our main goal was the fabrication of tunable plasmonic nanoparticles and the evaluation of their plasmonic performance as potential candidates for biomedical applications, such as biomedical sensing and imaging, drug delivery and plasmonic photothermal therapy.

WS2

P2-1 Surface Properties of Ceria Synthesised Using Triton-X Based Reverse MicroEmulsions
Charis R. Theocharis University of Cyprus, Cyprus

P2-2 Nanocellulose Containing Concretes: Evaluation of NC properties affecting UHDC & Development of Mixing Protocols
E. G. Deze API Europe, Athens, Greece

P2-3 Mesoporous Silica based copper catalytic materials: Synthesis, Characterization & deNOx Evaluation
E. G. Deze API Europe, Athens, Greece

P2-4 Influence of ITO thickness on the optical and electrical properties of the ITO/ZnO/glass bi-layers deposited by pulsed D.C. magnetron sputtering for chalcogenide photovoltaics
R.A. Mereu Babeş-Bolyai University, Romania

P2-5 Potential of silver nanoparticles in biological applications
Hochvaldova L. Palacký University Olomouc, Czech Republic.

P2-6 Novel Organically Modified Silica Nanoparticles for Dental Applications
A. Nikolaidis Aristotle University of Thessaloniki, Greece

P2-7 MOF-based carbon materials for enhanced electrochemical performance
K. Sielicki, West Pomeranian University of Technology, Poland

P2-8 Multiphoton Continuous Wave (CW) laser lithography enabling structuring beyond the diffraction limit
Theodoros Manouras Opticon ABEE, Greece

P2-9 The effect of glass surface modification on metal nanoparticles adhesion: thermal glass poling vs. chemical functionalization
TS. Selvam Ruđer Bošković Institute, Croatia

P2-10 Morphological changes of silicon nitride-based nanopowders prepared by two-stage spray pyrolysis method
H. Osip, AGH University of Science and Technology, Poland

P2-11 Synthesis of binary AlN/TiN nanopowders for no-additive high temperature and high pressure (HT-HP) sintering
H. Osip, AGH University of Science and Technology, Poland

P2-12 Direct oxygen content determinations in various non-oxide inorganic substrates used for the mechanochemical preparation of kesterite Cu2ZnSnS4 semiconductor
H. Osip, AGH University of Science and Technology, Poland

P2-13 Structural changes of titanium nitride TiN upon no-additive, high pressure and high temperature (HP-HT) sintering of nanopowders
J.F. Janik AGH University of Science and Technology, Poland.

P2-14 Silicon nitride-based nanopowders prepared by spray pyrolysis from selected organosilicon compounds
J. F. Janik, AGH University of Science and Technology, Krakow, Poland

P2-15 Elaboration of analytical methodology for direct determination of non-intentional oxygen contents in the semiconductor kesterite Cu_2ZnSnS_4 nanopowders
Jerzy F. Janik, AGH University of Science and Technology, Poland

P2-16 Hybrid nanostructures based on E.coli protein with iron oxide inorganic core
S.Yu. Turishchev, Voronezh State University, Russia

P2-17 Physico-chemical properties of nanocrystalline $LiFeGe_2O_6$
O. Skurikhina, Slovak Academy of Sciences, Slovakia

P2-18 Mechanochemical synthesis, characterization, and properties of Cu_2Se
Gáborová K., Slovak Academy of Sciences, Slovakia

P2-19 Iron oxide@graphitic carbon core-shell nanoparticles embedded in ordered mesoporous N-doped carbon matrix as an efficient cathode catalyst for PEMFC
Panagiotis Tsiakaras, University of Thessaly, Greece

P2-20 Enhanced electrocatalytic oxidation of urea-rich wastewater over novel bifunctional V_2O_3 nanosheets anchored N-doped-carbon encapsulated Ni heterostructure
Panagiotis Tsiakaras, University of Thessaly, Greece

P2-21 Electrocatalytic reduction of nitrogen: A simple strategy for continuous regulation of Faradaic efficiency by controlling H+ ions transfer rate
Panagiotis Tsiakaras, University of Thessaly, Greece

P2-22 Polymer / fly ash composites: Structure, morphology and dynamic thermomechanical properties
A. Stimoniaris, University of Western Macedonia, Greece

P2-23 Preparation by direct mixing and characterization of Graphene/poly(dimethyl siloxane) composites
P. Ketikis, National Technical Univ. of Athens, Greece

P2-24 Evidence of visible quantum cutting phenomenon in co-precipitation derived Eu3+ doped β-NaGdF4 nanorods
Y. Cheroura, Université Clermont Auvergne, France

P2-25 Surface and Wetting properties of Laser patterned Transition Metal Nitrides
M. Nousi, Nanotechnology Lab LTFN, Greece

P2-26 Coprecipitation synthesis and optical characterization of Tb^{3+}, and Tb^{3+}-Yb^{3+} doped □-$NaYF_4$ nanophosphors
Z. Smara, Université Clermont Auvergne, France

P2-27 Hyphenation of Field-Flow Fractionation and ICP-MS to overcome the size limitations of spICP-MS
Drexel R. Postnova Analytics GmbH, Germany

P2-28 Composite core-shell nanostructures synthesis by aerosol-assisted CVD
V.A. Klinkov Peter the Great St.-Petersburg Polytechnic University, Russia

P2-29 LbL films and microcapsules based on protamine and pectin-Ag nanocomposite
A. Hileuskaya Institute of Chemistry of New Materials of NASB, Belarus

P2-30 Growth of molybdenum sulphide ultra-thin films and their characterization
G. Papadimitropoulos NCSR “Demokritos”, Greece

P2-31 Laser annealing of amorphous molybdenum sulphide ultra-thin films
G. Papadimitropoulos NCSR “Demokritos”, Greece

P2-32 Morphological, structural, and electrical properties of vanadium oxide thin films
V. **Tsouti** NCSR “Demokritos”, Greece

P2-33 Synthesis of CoAl2O4 spinel coating by magnetron DC sputtering
D. Honcharenko Saint Petersburg Polytechnic University Russia

P2-34 Screen Printed Electrodes based on polymer/CNT and polymer/G nanocomposite for advanced gas sensing application
A. Grozdanov University Ss Cyril and Methodius in Skopje, Republic of North Macedonia

P2-35 Using carbon nanotubes based electrode in a two-chamber Microbial Electrolysis Cell for hydrogen production: comparison with conventional anode materials
G. **Antonopoulou** Institute of Chemical Engineering Sciences, Greece

P2-36 Catalytic activity of nanostructured carbon electrodes for electrosynthesis of H2O2 through water oxidation: Predictions from first principles
S. Piskunov, University of Latvia, Latvia

P2-37 Orientation imaging on grains within (La,Sr)MnO3 nanowires
M. R. Koblischka Saarland University, Experimental Physics, Germany

P2-38 1D crystal geometry optimization using evolutionary computations
T . Tarkowski University of Warsaw, Poland

P2-39 Carbon monoxide and nitric oxide reaction on oxidized Al-Mo(110) surface alloy: A model prototype of noble-metal based heterogeneous catalysis
T.T. Magkoev, North Ossetian State University, Russian Federation

P2-40 Effect of plasmonic gold nanoparticles on collagen
L. Draghiciu IMT Bucharest, Romania

P2-41 Ab-initio theoretical calculations and experimental synthesis of Sm1-xMMxCo5 (x = 0.1 – 1.0, MM = mischmetal)
G. Sempros Aristotle University of Thessaloniki, Greece

Surface Properties of Ceria Synthesised Using Triton-X Based Reverse MicroEmulsions

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The effect of the tail length of Triton-X surfactants on the surface properties of ceria prepared by means of reversed micelles and $Ce(OiPr)_4$ has been systematically studied. Generally, solids with increased surface areas (up to136 m^2/g) were synthesised.It was shown that the tail length strongly affects the surface characteristics. Further studies were carried out using UV-Vis, ATR-FTIR, XRD, TGA/DSC studies of the precursor gels as well as N_2-isothermal adsorption BET, XRD, FT-IR, UV-Vis Diffuse Reflectance and SEM investigations of the final solids samples. An interaction mechanism between the ceria precursor molecules and the polar tail of the reversed Triton X micelles and the formation of ceria (CeO_2) particles in the aqueous nucleus of the reversed microemulsions is proposed.

Nanocellulose Containing Concretes: Evaluation of NC properties affecting UHDC & Development of Mixing Protocols

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Cement composites represent one of the most widely used construction materials, but their brittleness or low strength properties often limit their applications. In recent years, scientific interest turned to the utilization of cellulose nanostructures (NCs) as concrete reinforcing agents. These novel materials considered to be promising candidates, capable of combining both cellulose properties and the unique features of nanomaterials. Within this context, API-Europe under ReSHEALience project aim to apply nanocellulose beneficial properties to Ultra High Durability Concretes (UHDC) technology. The main objective is to develop in-depth mixing protocols for the incorporation of cellulose nanoadditives into cementous blends. To this end, four different commercially available NC aqueous suspensions (two CNFs and two CNCs) were selected for the evaluation of the key aspects potentially affecting concrete final performance. Two of these samples were produced using AVAP® technology, whereas the other two were made with alternative processes. Incorporation of NCs into cementous mixture will offer a side-by-side performance comparison between CNCs and CNFs leading to a better understanding of particle morphology impact on composite properties. To further investigate the relationship between NC intrinsic features and material efficiency, a comprehensive analysis of both structural and physicochemical NC properties will also be accomplished through several characterization techniques (AFM, DLS, etc.). The as-obtained NC-enriched specimens will be tested and a correlation between strength and durability vs. nanocellulose properties will be obtained. In this way, proper selection of NC species along with fine tuning of additive content and fresh cement paste rheology will be feasible depending on manufacturer requirements. The optimal mixing procedure will be tested in two European pilot plants.

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Mesoporous Silica based copper catalytic materials: Synthesis, Characterization & deNOx Evaluation

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Over the last years, mesoporous silicas have gathered considerable interest especially in the field of de-NOx catalysis [1,2,3]. Amongst other, polyol process is considered a promising technique since a liquid polyol act as both solvent and reducing agent. In the present study, the development of catalytic systems was performed through a modified polyol route utilizing two mesoporous siliceous templates (MCM-41 & MCF-LA) as substrates and copper as the active component. The main objective was to investigate the effect of different textural characteristics on the development of MNPs and de-NOx catalytic activity. During the synthesis, microwave irradiation was applied as the heating source, whereas the size and dispersion of as-formed NPs on the porous hosts was effectively controlled through appropriate fine tuning of the different reaction parameters. Characterization results reveal the successful development of Cu NPs of 15 nm in size in all studied samples. Preliminary deNOx catalytic activity results under stoichiometric conditions demonstrate an enhanced performance reaching 35-40% maximum NO conversion by CO at moderate temperatures (~300 ^{o}C). However, a more detailed study is required for an in depth comprehension of the synthetic parameters that will enable the production of supported Cu NPs with desirable particle size distribution and enhanced catalytic activity.

Acknowledgement: The authors acknowledge the project entitled «*Development of a novel catalytic copper or/and palladium nanoparticles membrane for deNOx application*», with MIS 5047821.

References: [1] J. Zhu et al., Appl. Catal. B: Environm., 130, 197-217 (2013), [2] H. Song et al., J. Am. Chem. Soc., 128, 3027-3037 (2006), [3] E.G. Deze et al., Microp. Mesopor. Mater., 235, 107-119 (2016).

Influence of ITO thickness on the optical and electrical properties of the ITO/ZnO/glass bi-layers deposited by pulsed D.C. magnetron sputtering for chalcogenide photovoltaics

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In this work we compare the influence of the ITO thin film thickness in the glass/i-ZnO/ITO bi-layer structure used in CIGS thin film solar cell as a TCO bi-layer system. The characterization of the structures was done from the optical and electrical point of view. Apart from the basic physics of TCO materials our research had focused on the optimization of the deposition process. The development thus focuses on scaling up the processes on large areas and maximizing deposition rates and material utilization. In the approached deposition the main considered goal was the compatibility with industrial applications, namely this work refers to deposition of TCO films at moderate substrate temperature to the growth of ultra smooth high performance films with low thickness. Low resistivity (10-3 Ωcm) and high average transmission in the 400-800 nm range (≈88%) have been obtained for the bi-layer configuration. A special attention to the impact of the growth parameters like temperature, pressure and distance between the substrate and the target on the physical properties of the bi-layer was assigned.

Potential of silver nanoparticles in biological applications

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Silver nanoparticles of various size, shape, physical and optical properties might be prepared via different ways. Smaller the nanoparticle is, the higher surface area has, which results in an increased activity, coating ability, catalytic and antimicrobial activity, which has found many different uses in various applications. Most of the nanoparticles are prepared in colloidal form, but they can be also prepared as 2D films which are coated on different surfaces. Every silver nanoparticle has a unique surface resonance plasmon at the specific wavelength. The plasmon differs with the size and shape of the nanoparticle, which allows us to tune plasmonic properties and use them for signal enhancement in Raman or fluorescence spectroscopy. Silver nanoparticles are known for their high antibacterial properties against a broad range of bacterial species at concentrations ranging from a few ppm to tens of ppm which also do not have any cytotoxic effect to human cells. With the problem of increasing antibiotic resistance, new ways how to overcome it or postpone it are studied. One of the possible approaches is to use another antibacterial agent, which might be silver or other metal nanoparticles (Au, ZnO, Se NPs). However, since the bacteria were able to build up resistance towards antibiotics, it is expected to observe bacterial resistance even against to those nanoparticles. That has been recently confirmed for silver nanoparticles, but luckily at the same time new approach how to overcome this newly formed mechanism has been designed. Another way how to fight against resistant pathogens might be combination of antibiotics with silver nanoparticles, which might result in enhanced antibacterial activity even at substantially lower concentrations. It seems that the race between bacteria and scientists has begun, while each of them are forced to react to the newly developed mechanisms of their counterpart and respond to it as soon as possible.

Novel Organically Modified Silica Nanoparticles for Dental Applications

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In clinical practice, dental composite materials are constantly subjected to high force loadings, acidic factors and bacterial infections in the oral environment, thus still needing a more efficient enhancement by the addition of "multitasking" nanofillers. In the present study, three new methacrylated quaternary ammonium silanes (S.QAMs) were firstly synthesized through a variant of Menschutkin reaction between 2-(dimethylamino)ethylmethacrylate (DMAEMA) and a series of alkoxy silanes such as (chloromethyl)triethoxysilane, (3-chloropropyl)triethoxysilane and (chloromethyl)trimethoxysilane. The produced S.QAMs were characterized using proton nuclear magnetic resonance ($_1$HNMR) and Fourier-transform infrared spectroscopy (FTIR). Silica nanoparticles were then surface modified with the above S.QAMs by conducting a simplified silylation reaction under mild conditions. The structural characteristics of the obtained organomodified nanosilica were confirmed by means of FTIR and thermogravimetric analysis (TGA). These diverse S.QAMs structures are believed to further copolymerize with monomers of dental resins, resulting in a promising improvement not only of their physicochemical, mechanical and thermal performance, but also the antimicrobial activity of the dental nanocomposites due to the presence of bactericide ammonium

MOF-based carbon materials for enhanced electrochemical performance

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Today, the constantly increasing demand for energy is forcing scientists to develop and to design materials which can fulfil the expectations for high performance and low costs in energy storage and conversion. Therefore, the researchers currently are developing the materials, which are capable of storage high amounts of energy and converse the energy with high efficiency. To do that, many carbon-based materials were synthesised with focus on well-design and advanced structures. Many nanomaterials, beside sophisticated and well-defined structure, are doped with metal atoms or metal nanoparticles to increase the performance even higher. Promising materials which are well-known for one step-synthesis and large surface area are Metal-Organic Frameworks (MOF). The materials can be synthesised in hundreds of ways, with use of plenty of metals and organic linkers. That make the materials not yet completely defined and it grant a lot of space for further development.

One-step easy synthesis of the MOF materials, carbonization and modifications with Ni and Co metals were prepared. Analysis via variety of methods: TEM and SEM imaging, EDX mapping, X-Ray Diffraction, Specific Surface Analysis (via BET method), Raman Spectroscopy and Thermogravimetric Analysis has been provided. The electrochemical performance of the presented materials was tested for Hydrogen Evolution Reaction (HER) and due to profitable properties for Lithium-Ion Batteries as an anode electrode.

Multiphoton Continuous Wave (CW) laser lithography enabling structuring beyond the diffraction limit

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In this work, continuous-wave laser enabled multiphoton laser lithography processes and materials are demonstrated, using a CW diode laser source (375nm) to expose doped hybrid materials. The material formulations comprise proper dye molecules, which absorb in the exposing laser wavelength, where the matrix is transparent. If the radiation flux exceeds a certain threshold, the dye molecules initiate the structuring of the materials by the homolytic degradation of the acrylate bonds contained in the organic part. The non-linear nature of this process allowed features well below 500 nm to be generated. The laser structuring experiments were conducted on an in house manufactured X-Y Laser Exposure Tool. The combination of a non-linearly responsive material with a focused continuous laser beam lead to the creation of sub-diffraction limit structures. Furthermore, it was demonstrated that the dimension of the created structures can be defined by adjusting the power of the laser and the duration of the exposing laser pulse.

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Morphological changes of silicon nitride-based nanopowders prepared by two-stage spray pyrolysis method

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Silicon nitride Si_3N_4 and silicon oxynitride SiO_xN_y are important structural ceramics with many advantageous properties for technology. They can be prepared by a two-stage spray pyrolysis from suitable liquid organosilicon precursors. The raw products obtained in the first stage have spheroidal particle morphology typical for the method. In the second stage, an additional thermal annealing completes the changes towards stable products.

The goal of the study was to evaluate the impact of the first stage conditions and raw powder characteristics on the morphology of final powders. The liquid organosilicon compounds, triethoxymethylsilane and methytrimethoxysilane, were used as precursors. Ar gas was a transportation medium for the precursor mist into the tube reactor and NH_3 served as a nitridation reagent. The raw powders were produced at 1000, 1200, and 1400 °C. The thermal annealing in the second stage was carried out at 1400 °C under flowing ammonia.

The raw powders were amorphous as shown by XRD and had spheroidal morphology while FT-IR confirmed the presence of some Si–O groups. In the annealed powders, crystalline silicon oxynitride and amorphous silica were found. In the case of the raw powders made at 1400 °C, the spheroidal morphology was well preserved after second stage treatment. In other cases, fibre-like and/or fused features were observed instead. The morphology changes can be linked to the first stage processing conditions.

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Synthesis of binary AlN/TiN nanopowders for no-additive high temperature and high pressure (HT-HP) sintering

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Metal nitrides are advantageous materials for modern electronics and ceramics. Titanium nitride TiN is very hard and used in protective coatings of cutting tools while displaying electric conductivity higher than the metal. Aluminum nitride AlN is also hard and unique among insulators – has a very high thermal conductivity. Because AlN and TiN do not form solid solutions, no-additive high temperature and high pressure sintering of the nitrides nanopowders becomes the process of choice for making binary AlN/TiN composite materials.

The AlN/TiN nanopowders were prepared from an anaerobic organometallic precursor system. First, a hexane solution of a mixture of Al and Ti dimethylamides (Al/Ti = 1/1 at.) was prepared. After an equilibration stage (10 min at RT or 3 h-reflux), the hexane was evaporated and the finely mixed metal dimethylamides were reacted with liquid NH_3 (transamination/deamination) resulting upon evaporation of NH_3 in a solid mixture of the metals amide-imides as a precursor for nitridation. The precursor was pyrolyzed at 800-1100 ºC, 4 h, under an ammonia flow to yield the final binary nanopowders.

^1H NMR (C_6D_6) spectra of the mixed metal dimethylamides solutions in benzene revealed no reactions between the compounds. XRD patterns of the final nanopowders confirmed the presence of separate h-AlN and c-TiN phases with different average crystallite sizes in the nanosized range. Control of the pyrolysis conditions allowed for making the diverse binary nitride nanopowders for further HP-HT sintering.

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Direct oxygen content determinations in various non-oxide inorganic substrates used for the mechanochemical preparation of kesterite Cu_2ZnSnS_4 semiconductor

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The two-step mechanochemically assisted synthesis of kesterite Cu_2ZnSnS_4 – a perspective semiconductor for next generation photovoltaic cells – allows for a convenient, highly automated preparation of this complex sulfide. The first high-energy ball milling step yields a raw product with a high surface area and increased susceptibility to non-intentional oxidation (*e.g.*, handling in ambient air). The high temperature annealing in the second step results in conversion to the final tetragonal kesterite nanopowders with thermodynamically supported propensity for oxidation as well, which unfavorably modifies the crucial semiconductor properties. Our preliminary studies indicate that the kesterite nanopowders may at the end contain up to a few wt.% oxygen. In addition to adventitious oxygen sources during material processing and handling, some oxygen content in kesterite may have originated from the substrates. From this angle, the following solid precursors used by us to make kesterite nanopowders *via* different routes were tested for oxygen and hydrogen contents: elements (Cu, Zn, Sn, S), alloys (in situ made from the elements: Cu_6Sn_5 + Cu_5Zn_8), and metal sulfides (Cu_2S, CuS, ZnS, SnS, SnS_2). The oxygen-nitrogen-hydrogen Leco ONH836 analyzer was used for elemental analysis upon application of our elaborated methodology, which enables direct determinations of oxygen and hydrogen contents in all of these materials (Leco ONH836 is originally designed for O-content determinations in metals).

The determined oxygen contents range from a few tenths (metals, alloys) to a few percent (sulfides). This represents a significant share of the total oxygen content in the kesterite nanopowders.

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Structural changes of titanium nitride TiN upon no-additive, high pressure and high temperature (HP-HT) sintering of nanopowders

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TiN has a high hardness nearing that of diamond and electric conductivity higher than that of Ti-metal – a set of advantageous properties for modern electronics. The project's perspective is to make robust TiN nanoceramics *via* HP-HT sintering of nanopowders. Herein, reported are XRD and SEM results on TiN preparation and sintering. The synthesis route to nano-TiN is based on the ammonolysis chemistry utilizing the anaerobic precursor system $Ti[N(CH_3)_2]_4/NH_3$ and pyrolysis of Ti-imide under NH_3 (800 and 1100 °C, 4 h – dark brown powders). Based on XRD, cubic TiN is prepared, *i.e.*, c-TiN(800 °C): a = 4.236 Å, D_{av} = 10 nm; c-TiN(1100 °C): a = 4.241 Å, D_{av} = 57 nm. SEM confirms that nanopowders are made of agglomerated particles.

Sintering is performed at 7.7 GPa, 3 min, at two temperatures: 650 °C that is lower and 1200 °C that is higher than both powder preparation temperatures with the latter anticipated to promote recrystallization. From the XRD data, the nanoceramics are made of cubic TiN. For sintering TiN(800 °C) nanopowder at 650 °C: a = 4.238 Å, D_{av} = 8 nm, and at 1200 °C: a = 4.250 Å, D_{av} = 21 nm. For sintering TiN(1100 °C) nanopowder at 650 °C: a = 4.237 Å, D_{av} = 13 nm, and at 1200 °C: a = 4.243 Å, D_{av} = 30 nm. Sintering at 650 °C demonstrates the impact of high pressure by decrease of the average crystallite sizes D_{av} of both nanopowders – nanocrystallite crushing phenomenon in the absence of recrystallization. Sintering at 1200 °C results for powder TiN(800 °C) in a higher D_{av} whereas for powder TiN(1100 °C) in a lower D_{av}, relatively, the latter outcome being a compromise of adverse actions of P and T on particle size.

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Silicon nitride-based nanopowders prepared by spray pyrolysis from selected organosilicon compounds

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Silicon nitride Si_3N_4 and silicon oxynitride SiO_xN_y have many advantageous properties for technology. There are several routes known for preparation of the nitrides nanopowders including spray pyrolysis from liquid precursors. In favorable cases, the precursor mist is transported with an inert gas, or a mixture of gases, through a preheated tube reactor to undergo complex changes before reaching the exhaust filter. Due to short residence times in the hot zone, the pyrolysis reactions may not be completed and the raw powders obtained in this stage require an additional treatment at suitable temperatures and gas atmosphere.

The goal of the study was to test the impact of gas atmosphere in the first stage of spray pyrolysis on the composition of raw powders. Oxygen-bearing liquid organosilicon compounds, polydimethylsiloxane (PDMS) and methyltrimethoxysilane, were used as precursors. The runs were carried out at 1200 and 1400 °C under various gas atmosphere conditions. First, Ar/NH_3 was used for mist transportation and as a reaction gas and, second, neutral N_2 was applied. XRD results confirmed that all powders were amorphous while SEM showed spheroidal particle morphology typical for the process. The powders made in Ar/NH_3 were creamy-white while those made in the N_2 atmosphere were blackish. The O and N contents measured by LECO ONH836 analyzer showed the impact of temperature on powder composition (*e.g.*, for PDMS at 1200 and 1400 °C, respectively, O - 4.9 wt%, N - 21.7 wt% and O - 11.1 wt%, N - 22.0 wt%). FTIR spectra confirmed the presence of the Si–N and Si–O bonds in the powders made in the Ar/NH_3 atmosphere whereas N_2 promoted Si–O bond formation.

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Elaboration of analytical methodology for direct determination of non-intentional oxygen contents in the semiconductor kesterite Cu_2ZnSnS_4 nanopowders

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Semiconductor properties of kesterite Cu_2ZnSnS_4 – considered for next generation of photovoltaic cells – crucially depend on stoichiometry and structure characteristics including site substitutions and vacancies. Due to high specific surface area, in addition to adsorption of gases, kesterite nanopowders can react with oxygen O_2 and water vapor H_2O to form metal-O and sulfur-O moieties as well as -OH species if exposed to air. This and other uncontrolled processing factors contribute to adventitious oxygen contents.

Until recently, no direct determination of oxygen forms in inorganic materials has been available due to analytical limitations. Herein, presented are first attempts of this kind for kesterite using the state of the art oxygen-nitrogen-hydrogen analyzer (Leco ONH836) and an originally elaborated methodology. Under suitable instrumental and analytical conditions, the latter enables determinations of different O-forms. Kesterite was prepared by a two-stage mechanochemical route consisting of high-energy ball milling of the metal sulfide precursor system (Cu_2S+ZnS+SnS+S) in a planetary ball mill and annealing at 500 and 550 °C, 6 h, Ar. The phase composition of the materials was studied with powder XRD, semiconductor properties were determined by UV-vis spectroscopy, and oxygen contents were measured with the Leco analyzer.

The results show that the total O-contents may reach levels of a few wt%. This is oxygen mainly associated with chemisorbed H_2O and/or with -OH groups. Some oxygen originates from metal oxides and, possibly, sulfates formed on particle surfaces upon non-intentional while significant oxidation processes in air. The presence of sulfates introduces complications and forces further refinements of the methodology.

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Hybrid nanostructures based on E.coli protein with iron oxide inorganic core

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Dps protein of Escherichia coli (E.coli) belongs to the ferritine-like group and represents a nanoscale hybrid particles consisting of 9 nm organic shell and 5 nm inorganic core. The protein shell is formed by a twelve identical subunits with the known structure as a dodecamer.

In present paper the direct experimental information about specificity of iron atoms local surrounding in ferritines immobilized into planar and nanostructured silicon surfaces using a soft X-ray synchrotron radiation spectroscopy have been applied. Additionally, high resolution cryo-transmission electron microscopy, AFM, dynamic light scattering have been performed. The thermal and ion beam treatments were used for surface modification. The presence of both Fe2+ and Fe3+ ions in the octahedral and tetrahedral surrounding of O atoms in the Dps protein samples consisted of ~10 nm hybrid particles with ~5 nm inorganic cores were observed. Partial Fe restoration followed by the surface post treatment is shown revealing a complex composition of the hybrid particles cores even in the native Dps protein, that has been isolated from aerobically grown bacteria. These proteins containing inorganic iron-oxygen nanoparticles can be considered perspective for a novel low-cost and energy effective technology for the functional low-dimensional materials formation.

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Physico-chemical properties of nanocrystalline $LiFeGe_2O_6$

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$LiFeGe_2O_6$ (lithium ir $LiFeGe_2O_6$ (lithium iron methagermanate) is a complex oxide from pyroxene family that is extensively studied regarding its interesting crystal and magnetic structures (Nestola, Redhammer, Pamato, Secco, & Dal Negro, 2009; Redhammer et al., 2009). Possible application of carbon composites based on pyroxenes was investigated respecting their use as cathode materials for Li-ion batteries. However, the stiffness of the structure hampered delithiation–lithiation process (Ni et al., 2010).

In this work, the influence of two different Fe^{3+} precursors, i.e., α-Fe_2O_3 (hematite) and α-FeO(OH) (goethite), on the synthesis of $LiFeGe_2O_6$ is studied. The formation process of the complex oxide was accelerated and simplified by the high-energy ball milling and completed during the subsequent thermal treatment. Although the as-synthesized materials, studied by X-ray diffraction and ^{57}Fe Mössbauer spectroscopy, showed one-phase product in both cases, a slight color difference between the two samples was observed. To increase the diffusion rate of Li^+ in the as-prepared phase pure $LiFeGe_2O_6$, the material was additionally milled with an aim to amorphize it. This was motivated by the fact that the comminution of particles can accelerate diffusion process and can enhance electrochemical performance of materials. Furthermore, oxides in a far-from-equilibrium state can possess diverse structural features such as spin canting, re-arrangement of cations, etc. (Sepelak, Begin-Colin, & Caer, 2012).

Mechanochemical synthesis, characterization, and properties of Cu_2Se

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Selenium compounds are relatively rare as minerals. One of them is berzelianite with a chemical formula Cu_2Se which has unique optical and electrical properties. Therefore, many different methods have been reported for synthetic copper(I) selenide (Cu_2Se) powder preparation. Synthetic Cu_2Se, a potential candidate for green energy devices, is a typical p-type semiconductor suitable for solar cells and thermoelectric materials[2]. In our study, we suggest environmentally friendly and fast approach for Cu_2Se synthesis. Nanostructured Cu_2Se was synthesized via one-step mechanochemical synthesis after 5 min milling in a planetary ball mill, Pulverisette 6 (Fritsch, Germany) under Ar-atmosphere. A gradual course of synthesis was followed by the gas pressure and temperature measuring system (GTM). The product was characterized by X-ray diffraction, specific surface area measurements, particle size distribution, X-ray photoelectron spectroscopy, scanning, and transmission electron microscopy. The X-ray diffraction confirmed the orthorhombic crystal structure of Cu_2Se (JCPDS PDF 047-1448). The binding energy values of the Cu 2p and Se 3p signals from the XPS spectrum correspond to Cu^{1+} and Se^{2-} oxidation states in the product. The optical properties were studied using UV-Vis and photoluminescence spectroscopy. The value of direct band gap energy 3.7 eV was obtained based on the recorded optical absorption spectrum in a UV–Vis spectral region.

Iron oxide@graphitic carbon core-shell nanoparticles embedded in ordered mesoporous N-doped carbon matrix as an efficient cathode catalyst for PEMFC

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Most of the research work until nowadays for oxygen reduction reaction (ORR) in polymer electrolyte fuel cell (PEMFC) has focused on non-precious-metal catalysts (NPMCs) in basic media. In this work, we synthesized FeO_x@graphitic carbon core-shell structured nanoparticles implanted in N-doped carbon matrix with ordered and mesoporous structure (FeO_x@GC-NOMC) as an efficient cathode catalyst for PEMFC. This hybrid exhibits a highly 4 electron selectivity towards ORR, better electrocatalytic activity ($E_{1/2}$=0.81 V vs RHE) and superior stability and tolerance to methanol compared with commercial 20 wt.% Pt/C ($E_{1/2}$=0.77 V vs RHE). These features are attributed to the order mesoporous carbon matrix (promotes the rapid transfer and active sites exposures and limit the embedded nanoparticles size and hinder its agglomeration), the high content of ''Fe-N'' active sites and the core-shell structure of embedded nanoparticles (FeO_x@GC) (helps to avoid the corrosion of the active sites and ensures the long-term durability). Among the tested catalysts and currently reported NPMCs, the as prepared FeO_x@GC-NOMC presents one of the best H_2-O_2 PEMFC single-cell performances with a peak power density up to 350 W g^{-1} (1050 mW cm^{-2} based on active area). Moreover, it exhibits good long-term durability with a slight current decay after a chronoamperometric test of 120 h.

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Enhanced electrocatalytic oxidation of urea-rich wastewater over novel bifunctional V2O3 nanosheets anchored N-doped-carbon encapsulated Ni heterostructure

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In this work, we synthesize the V_2O_3 nanosheets anchored N-doped-carbon encapsulated Ni heterostructure (Ni@C-V_2O_3/NF), which is verified by SEM, TEM, XRD, and XPS and tested for the reactions of urea oxidation (UOR) and hydrogen evolution (HER). The electrochemical results indicate that the as synthesized material exhibits small potentials of 1.32, 1.39, and 1.43 V for UOR and small overpotentials of 36, 254 and 355 mV for HER at 10, 500 and 1000 mA cm^{-2}, respectively. A current density of 200 mA cm−2 is produced for over 50 h with negligible reduction of performance. Additionally, in order to evaluate the electrochemical performance of Ni@C-V2O3/NF for overall urea-oxidation, we use it as anode and cathode in urea electrolysis. When used for both cathode and anode electrodes, it can be stable at a current density of 100 mA cm−2 for over 70 h without erosion, emphasizing the stability. The reason could be attributed to collaborative effects between Ni and V, N-doped-carbon coating structure, and nano/micro nanosheets architecture self-supported on nickel foam. This work could provide a promising, cheap and green method for the degradation of urea-rich wastewater and hydrogen production.

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Electrocatalytic reduction of nitrogen: A simple strategy for continuous regulation of Faradaic efficiency by controlling H+ ions transfer rate

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Abstract Electrocatalytic nitrogen reduction (NRR) is almost an ultimate way to produce active nitrogen for agriculture, and high-energy-dense carbon-free fuels for our blue planet. The ammonia produced by Haber–Bosch process enhances the crop's ability to absorb carbon dioxide, increases grain production and that way supports almost half of the world's population today. However, the output efficiency of NRR is greatly limited due to the competitive hydrogen reduction reaction, which leads to extremely low faradaic efficiency (FE). The H^+ ions transfer rate can be controlled by regulating the pore area of membrane; there is a nearly linear relationship between those two at a suitable voltage. The proportion of H^+ ions involved in NRR is relatively small, so the NRR is less affected when the pore area is reduced, but FE is significantly increased. In this work, a physical model describing FE and H+ ions transfer rate is established, which matched well with the experimental data in a wide range. FE can be continuously regulated by changing the pore area of membrane, achieving the highest FE of 41.86 % (from 9.04 %) with the surface plasmon-enhanced FeAg nanoclusters at -2.13 V in a two-electrode photoelectric system. This physical model is also applicable to many other ways of improving the FE, and a wide range of applications can be derived from it.

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Polymer / fly ash composites: Structure, morphology and dynamic thermomechanical properties

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Thermoset and thermoplastic polymer composites with fly ash as filler have attracted considerable interest due to their inherent good mechanical properties and low cost [1-2]. In this study the morphology and the dynamic mechanical properties in polymers/fly ash and their composites are outlined. Pristine fly ash and that modified with organosilanes of the type $(RO)_3SiCH_2CH_3$ is incorporated into epoxy resin DGEBA (thermoset) and polystyrene-b-polybutadiene (PS-b-PB, thermoplastic) matrices is used [3]. Details for sample preparation are presented elsewhere [4]. Scanning electron microscopy (SEM) was used to clarify the dispersion, the distribution and the degree of aggregation/agglomeration of fly ash particulates in the matrix. DMA, DSC and TGA measurements show a clear dependence of the dynamic properties of the composites on the filler loading, the surface modification and the matrix nature [5]. In addition, the thermogravimetric curves are also employed to characterize the heat-resistant performance of the composites. Special attention has been given to the mechanism of thermal transport and diffusivity. Additionally, the influence of interface between matrix and filler on the dynamic thermomechanical properties is examined. These results, along with those published by other researchers [1] show that these materials can be successfully used for long scale applications. A recent application of these materials is the preparation of thick plasters used in the thermal insulation of buildings.

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Preparation by direct mixing and characterization of Graphene/poly(dimethyl siloxane) composites

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Polydimethylsiloxane (PDMS) has been widely used in various industrial fields due to its nontoxicity, biocompatibility, low cost, ease of fabrication and electrical insulating properties. However, due to its poor mechanical properties, there are significant limitations in its applications and therefore is usually reinforced with fillers. Graphene (GN) nanoplatelets, due to their unique properties, such as excellent thermoelectrical conductivity and mechanical properties, are a promising reinforcing filler for polymer composites with a vast range of applications in automobile industry, aerospace, solar cells actuators, batteries and sensors.

The present study investigated the effect of GN nanoplatelets on the properties of PDMS composites, prepared by direct mixing using sonication. The calculation of D (1350 cm^{-1}) and G (1580 cm^{-1}) bands ratio (I_D/I_G), recorded by RAMAN spectroscopy, suggested an increase in carbon defects, when graphene was incorporated in the PDMS matrix. The effect was attributed to the sonication procedure applied to the mixture. The thermal stability of the composites deteriorated, especially for higher GN concentrations (0.8 and 1 phr), as detected by thermogravimetric analysis (TGA). As to their mechanical properties, the tensile strength was enhanced up to 69% for composites reinforced with 0.5 phr GN. The elongation at break increased for all composites, along with the modulus of elasticity, which improved especially at higher GN content (0.5 and 0.8 phr). The incorporation of GN nanoplatelets affected the elastomeric network, restricting the swelling of specimens immersed in toluene, especially for the 0.5 phr GN composite. Membranes of PDMS composites reinforced with 0.5 phr and 1 phr GN, exhibited a decrease in oxygen permeability of 28% and 53% respectively, in comparison with unreinforced PDMS specimens.

Evidence of visible quantum cutting phenomenon in co-precipitation derived Eu^{3+} doped β-$NaGdF_4$ nanorods

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Pure hexagonal β-NaGdF4 and Eu3+ doped β-NaGdF4 nanocrystals in shape of nanorods of ∼140 nm of length have been synthesized using a simple and rapid coprecipitation method (1 hour at 150 0C) [1]. XRD analysis evidenced pure single phases exhibiting characteristic luminescence of Eu3+ ions when excited under VUV-UV radiations. Samples gave rise to good internal quantum yield efficiencies and an intense orange-red emission. Optical properties are discussed in the frame of Judd-Ofelt theory [2] and considering that an energy transfer occurs between active ions. Notably it was found that near-VUV excitation in the Gd3+ excited states, leads to quantum-cutting by Down-Conversion, which is realized through a two-step energy transfer from Gd3+ to Eu3+. Such process improves the intensity of the red emission of Eu3+ ions. However, the efficiency of this process in comparison with existing works in the literature [3] suggest that only one part of the energy in the excited states within Gd3+ can be transferred to Eu3+ for its red emission.

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Coprecipitation synthesis and optical characterization of Tb^{3+}, and Tb^{3+}-Yb^{3+} doped □-$NaYF_4$ nanophosphors

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Cubic □-NaYF4 nanometer-sized crystals doped with Tb3+, or Yb3+-Tb3+ ions were synthesized by an original coprecipitation route [1]. The obtained nanoparticles exhibited primary particles showing cubic shape with sizes ranging between 35 and 65 nm. Structural and morphological properties of the samples were analyzed by X-Ray Diffraction (XRD) and Transmission Electron Microscopy (TEM). The nanophosphors showed intense ultraviolet (UV) or near infrared (NIR)-excited green (Tb3+) emissions, which resulted from down- or up-conversion processes occurring in their structure. The concentration quenching of the Tb3+ ions emission in singly doped or Yb3+ co-doped □-NaYF4 were ascribed to resonant cross-relaxations. The main interaction between the active ions was evidenced as an electric dipole-dipole one through fitting the decays curves with the Inokuti-Hirayama model [2]. The critical distances and energy transfer microparameters for the transfer processes were determined, indicating a very short interaction range. The dependence of integral up-conversion intensity on the NIR energy of the beam power was measured. The results indicated a two-photon process based on cooperative energy transfer.

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Composite core-shell nanostructures synthesis by aerosol-assisted CVD

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Formation of core-shell particles causes significant scientific resonance. Existing technologies are complicated, multi-stage, not always allow getting core-shell type material, rather than mixture. In this connection, it is clear that the technological process in which the formation of core-shell nanostructures with variable characteristics that is carried out in single reaction volume is of great interest. The aim of this work was developing a simple technological solution in which it is possible to obtain core-shell nanoparticles with controlled characteristics and high rate. We used aerosol-assisted CVD method, in which solution of shell-forming component with dispersed nanoscale core-forming component was the reagent. Aerosol was created by piezoelectric nebulizer and transferred into a “hot walls” tubular quartz reactor for shell-forming component pyrolysis, the deposition zone was located downstream. The carrier gas flow rate (He, Ar) was determined by the reagents pyrolysis time. Electrostatic filter was used to collect nanoparticles. The proposed method has been tested to obtain “core Fe_3O_4-shell C” and “core Cu(Au)-shell MoS_2” nanostructures which are promising materials for medicine, sensorics, battery industry, etc. For the first, magnetic fluid with magnetite nanoparticles (about 10 nm) based on DMF with dissolved benzoic acid was used. For the second, pre-synthesized Cu (Au) nanoparticles (units of nm) in DMF and $(NH_4)_2MoS_4$ were used. By adjusting the process parameters, core-shell particles of tens to hundreds nanometers scale with a narrow size distribution were obtained, what was confirmed by SEM, HR TEM and Raman spectroscopy. The method is general to obtain different core-shell nanostructures in a gas stream with high rates. It is possible to use compounds that decompose before sublimation. Variations of process parameters allow smooth and predictable changing of the obtained particles structural characteristics.

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Surface and Wetting properties of Laser patterned Transition Metal Nitrides

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Artificial biomimetic surfaces and materials are inspired by the nanostructures that nature develops through the evolution process such as the superhydrophobic lotus leaf, the antibacterial shark skin among others. In this work we are using short and ultrashort pulsed laser beams processes for the fabrication of biomimetic surfaces based on transition metal nitrides (TMN) and we study their wetting properties.

The TMN biomimetic surface is fabricated via a two-step process. Firstly the TMN coating (thickness > 300 nm) is grown of top of silicon and stainless steel substrate, and then a Nd:YAG picosecond laser with multiple harmonics(1064 and 532 nm) is used to for the partial ablation and fabrication of the TMN surface. Several TMNs are studied in this work such as the well-studied Titanium Nitride as well as several emerging ternary TMNs, such as the $Ti_{1-x}Mg_xN$, $Ti_{1-x}Sc_xN$ and $Ti_{1-x}Ca_xN$.

Atomic Force Microscopy was used to study the surface morphology of the TMN surface patterns after the LA process, while the wetting behavior of the TMN surface was studied by Contact Angle. The surface scanned area was 20×20 nm and the RMS (Sq) surface roughness value for TiN was 16.3 nm, for $Ti_{1-x}Mg_xN$ with different Mg contents ranges from 39.8nm to 47 nm, while for the $Ti_{1-x}Sc_xN$, $Ti_{1-}xCa_xN$, the Sq was 26.5 nm and 77.5 respectively. The TMN surface wetting properties was studied by measuring the water droplet contact angle on top of the TMN surface and analyzing it based on the Wenzel’s theory, while the results are correlated with the surface roughness.

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LbL films and microcapsules based on protamine and pectin-Ag nanocomposite

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Nanocomposites based on silver nanoparticles and biopolymer are promising materials for biomedical application due to their antimicrobial potential. The aim of this work was to design of LbL-films and microcapsules based on pectin-Ag nanocomposite (AgNC) and protamine (PtS) suitable for antimicrobial surface protection and theragnostic applications. Biocompatible AgNC with strong antimicrobial properties was previously synthesized by «green» chemistry method. The physico-chemical properties of (PtS/AgNC)n multilayers were investigated by QCM and AFM methods. (PtS/AgNC)n multilayers were also tribologically tested. It was determined that LBL-films formed from aqueous solutions of polymers are elastic (μ=1.06 MPa) and have thickness of 67.1±9.3 nm, while using of polymer solutions in 0.15 M NaCl resulted in the formation of more viscous (μ=0.31 MPa) films with a thickness of 410.8±88.4 nm. We have also design of (PtS/AgNC)n microcapsules (MCs) based on the same biopolymers. For MSc fabrication, polymers had been layered on the 5 μm $CaCO_3$ core, which was subsequently dissolved by HCl. To perform *in vivo* biodistribution experiments, the surface of MCs was modified due to 1) arginine residues (NH_2-groups) of protamine layer exposed on the surface of MCs from under pectin-Ag layer using Cy5.5 NHS ester and 2) carboxylic groups of the terminal pectin layer using Cy5.5 amine derivative and EDC/NHS coupling reaction. Due to the abundance of carboxylic groups on the surface, the MCs modified by Cy5.5 amine derivative had stronger fluorescence emission compared to MCs modified by Cy5.5 NHS ester. The new Cy5.5-MCs are to be tested for *in vivo* biodistribution in the future.

Growth of molybdenum sulphide ultra-thin films and their characterization

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In this work a simple method for depositing MoS_2 ultra-thin films is described. The deposition system is equipped by a rotated shutter system which enables the deposition of MoS_2 films with thicknesses from a few monolayers to some nanometers. Amorphous MoS_2 films (a-MoS_2) were deposited by heating a molybdenum wire at low temperatures, between 300 and 450 ^oC in an ambient composed by H_2 and H_2S. Both H_2 and H_2S flows were 4 sccm, fixing the deposition pressure at 1,5 Torr. During deposition the samples remained at room temperature, rendering this deposition technique suitable for organic and plastic substrates. The deposited films were also subjected to thermal and microwave annealing and were characterized with various techniques to investigate the interplay between the adopted processing conditions and the resulting chemico-physical properties. SEM and AFM analysis revealed the smooth and fine grained surface of the samples. X-ray microanalysis has shown that the presence of H_2 during deposition results in a significant decrease of O and C contamination. XRD measurements revealed the amorphous character of the samples. Microwave annealing (in contrast to thermal annealing) at a power of 800 W seems to improve the atomic ordering in films, therefore XRD peaks corresponding to MoS_2 start to rise. The Raman spectrum have shown the sharp E_{2g} and A_{1g} peaks at 383,8 cm^{-1} and 408 cm^{-1}, respectively, typical for MoS_2, which compared with those of amorphous material are now stronger and narrower. Summarizing, a simple method for depositing MoS_2 ultra-thin films at room temperature was presented. The as deposited films were amorphous and were characterized with respect to their morphology and chemical composition.

Laser annealing of amorphous molybdenum sulphide ultra-thin films

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Abstract:

The MoS_2 ultra-thin films are deposited very easily by heating a molybdenum wire (in combination with a rotated shutter system) at low temperatures and in an ambient composed by H_2 and H_2S. The deposited films are amorphous, as shown using XRD and Raman measurements, which is a disadvantage for their electronic properties and their use in high quality thin film transistors.

Laser annealing of amorphous MoS_2 layer, for its thermally induced crystallization, offers significant advantages with respect to more conventional thermal annealing or curing techniques (e.g. oven). Apart from the obvious lateral selectivity, the use of short-pulsed and high repetition rate lasers minimizes the heat affected zone and offers unparalleled control over a digital process, enabling the processing of stacked and pre-structured layers on a variety of substrates.

In this work a nanosecond pulsed laser with a wavelength at 532 nm was used, operated at 100 kHz and combined with a 2D galvanometer scan head (max scanning speed 5 m/s) in order to irradiate the amorphous MoS_2 film in a homogenous manner on different substrates (Si, SiO_2 and metallic pads on Si). The influence of the laser power on the crystallization of the MoS_2 layer was investigated by characterizing the irradiated surface with Raman spectroscopy and XRD. For the three different substrates, the laser power values for the optimal possible crystallization differed (1, 1.5 and 3 W for SiO_2, metallic pads and Si respectively), implying an effect due to the different thermal characteristics of these substrates.

Morphological, structural, and electrical properties of vanadium oxide thin films

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Abstract:

Vanadium oxide films were chemically vapor deposited (CVD) on oxidized Si substrates covered with CVD tungsten (W) thin films and on glass substrates covered with indium tin oxide (ITO) films, using vanadium(V) oxy-tri-isopropoxide ($C_9H_{21}O_4V$) vapors. The surface morphology was studied with atomic force microscopy (AFM) and scanning electron microscopy (SEM). These measurements revealed that the morphology strongly depends on the used substrate and the deposition conditions. X-ray diffraction (XRD) measurements showed that the deposited films were composed of a mixture of vanadium oxides; the composition was determined mainly by the deposition temperature and less by the precursor temperature. At temperatures up to 450 ^oC the films were mostly composed by monoclinic VO_2. Other peaks corresponding to various vanadium oxides were also observed. X-ray microanalysis confirmed the composition of the films. The well-known metal-insulator transition was observed near 75 ^oC for films mostly composed by monoclinic VO_2. Films deposited at 450 ^oC exhibited two transitions one near 50 ^oC and the other near 60 ^oC possibly related to the presence of other vanadium phases or of important stresses in them. Finally, the vanadium oxide thin films exhibited significant sensory capabilities decreasing their resistance in the presence of hydrogen gas with response times in the order of a few seconds and working temperature at 40 ^oC.

Synthesis of $CoAl_2O_4$ spinel coating by magnetron DC sputtering

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Abstract: Cobalt aluminum spinel ($CoAl_2O_4$) is widely used in various applications such as detectors, thank to luminescence, optical, sensing and dying properties, high thermal and chemical stability, high catalytic activity. Different methods are known to synthesize this material, such as wet chemical method, co-precipitation, sol–gel method etc. In this paper $CoAl_2O_4$ coatings were successfully obtained by magnetron DC sputtering and subsequent oxidation. The process conditions have been optimized using calculated dependence of incoming particles energy assuming ballistic trajectories. The deposition profile was calculated using SimTra software, which allows us to establish relationship between process time and rotation rate for the best materials distribution on the substrate surface. Variation of the deposition power and duration of the process control phase composition, which yield to shift of the absorption band position on the spectrum. Obtained coatings can be used as optical filters. The films show high heat resistance in air (no less than 1573 K) and chemical resistance to H_2SO_4, HCl, HNO_3 but dissolve in HF. This research work was supported by the Academic Excellence Project 5-100 proposed by Peter the Great SPbPU "Development of glassy and composite materials for biosensors and smart medicine devices"

Screen Printed Electrodes based on polymer/CNT and polymer/G nanocomposite for advanced gas sensing application

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In order to prevent or minimize the damage caused by atmospheric pollution, monitoring and control systems are needed that can quickly and reliably detect the quantify sources of pollution within the range of regulatory standard values. Successful implementation of such a system is enabled using gas sensors. The main goal of this work is to obtain nanocomposite-based sensors from biocompatible polymer - polyethylene glycol (PEG) and conductive polymer - polyvinylidene fluoride (PVDF) reinforced with carbon nanostructures designed for the detection of gas oils. Also, 3D printing was used to modify SPE with Polylactic acid. The research was carried out in three phases. The first phase was followed by the change in the resistance of the commercial electrodes, by exposing the sensor to ammonia vapors of varying concentrations. In the second phase, the polymers (polyethylene glycol (PEG) and polyvinylidene fluoride (PVDF)) were applied by the drop method, i.e. drop modification method on the sensor electrode and the change in resistance of the sensor to exposure to ammonia vapor with varying concentration is monitored again. In the third phase, the characterization of the nanocomposite film was performed after the sensor measurements. Resistivity variations were found for different acid as well as base concentration. Surface changes of the SPE-sensors, before and after acid exposure, were followed by SEM. Polymer/CNTs interactions and their changes due to the gas vapors were studied by FTIR-ATR spectroscopy. SEM photos have shown formation of typical nano-rods of oxides.

Using carbon nanotubes based electrode in a two-chamber Microbial Electrolysis Cell for hydrogen production: comparison with conventional anode materials

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Abstract: In the present study two identical two-chamber Microbial Electrolysis Cells (MECs) (MEC1 and MEC2) were used for hydrogen production, using as bio-catalysts mixed anaerobic microbial consortia. For both MECs, the cathode (counter) electrode was made of carbon cloth coated with a Pt catalyst (ETEK, 0.5 mg/cm^2), while the anode (working) electrode was made of different materials: i.e. for MEC1 it was made of commercial carbon fiber paper while for MEC2, carbon nanotube (CNT) buckypaper was used. CNT buckypaper was prepared using multiwalled carbon nanotubes (MWCNTs) produced using the catalytic chemical vapor deposition method (CCVD) of hydrocarbon sources on substrates of metal oxides, impregnated with metal catalysts (Fe and Al). Chemical functionalization of CNTs with carboxyl (–COOH) was performed (MWCNTs-COOH) since the introduction of carboxylic acid groups on the surfaces of the NT improves their hydrophility. Characterization of CNT backypaper through Raman Spectroscopy, Scanning Electron Microscopy (SEM), and Brunauer–Emmett–Teller (BET) was carried out.
Both MECs operated at 30^{o}C, at control electrode potential (0.9 V) in a draw and fill mode, using synthetic acetate medium. During the first cycle of operation of the MECs, enrichment of the anodic electrodes with electrochemically active bacteria was performed, while during the subsequent cycles of operation hydrogen evolution was observed. MEC2 exhibited higher hydrogen production efficiency (rate and yield), higher organic matter removal efficiency and current production. Electrochemical characterization through Cyclic Voltammetry, chronoamperometry and Impedance Spectroscopy (Nyquist and Bode plots) was carried out and the MEC performance was correlated with the biochemical and electrochemical characteristics of the cells.

Catalytic activity of nanostructured carbon electrodes for electrosynthesis of H_2O_2 through water oxidation: Predictions from first principles

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Abstract: H_2O_2 is a widely used reactant in industry, and a perfect agent for waste water treatment and drinking water preparation. H_2O_2 production via the electrocatalytic two-electron water oxidation reaction (2e WOR) is preferable to the presently used anthraquinone industrial process. The main challenge is to achieve selectivity of 2e WOR versus the competing 4e WOR which results in the O_2 gas evolution. At the moment the reaction conditions for selective 2e WOR remain mainly unknown, even though, different metal oxide electrodes, i.e. ZnO, MnO_2, SnO_2, WO_3, TiO_2, IrO_2, $BiVO_4$, were studied both theoretically and experimentally. Even though, some materials exhibited catalytic activity, further search for a better catalyst is still actual, due to limited chemical stability in aggressive H_2O_2 media and/or lack of selectivity.
In our study the carbon-type nanostructured electrodes for 2e WOR were studied from first principles by means of density functional theory. Calculated free energy of 2e WOR intermediates' adsorption and calculated overpotential required for successful 2e WOR are used as descriptors for comparing carbon-type thin films, their possible morphologies and reconstructions. The results are presented in both free energy diagrams and the volcano plot diagrams for graphene, bilayer graphene, diamond, and B-doped diamond. Our study provides deeper understanding of the catalytic properties of the carbon allotropes and influence of dopants on 2e WOR. Funding from European Union`s Horizon 2020 Research and Innovation Program project under grant agreement No 768789 is greatly acknowledged.

Orientation imaging on grains within (La,Sr)MnO_3 nanowires

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The microstructural properties of electrospun, ferromagnetic La0.8Sr0.2MnO3 (LSMO) nanowires were investigated by means of orientation imaging. Fragments of the resulting nanowire network fabrics are placed on a carbon-coated TEM grid, and the grids are mounted on a customized sample holder which allows for investigations in the standard reflection electron backscatter diffraction (EBSD) and transmission Kikuchi diffraction (TKD) mode without breaking the vacuum. In this way it is possible to obtain crystallographic orientation maps of the LSMO grains within an individual nanowire section. The diameter of the LSMO nanowires is about 200 nm, whereas the size of the LSMO grains within the nanowires is typically in the 10-20 nm range. Our analysis shows that the nanowires can be as thin as a single LSMO grain. In this case, one can employ the TKD technique directly, which considerably enhances the Kikuchi pattern quality required to enable an automated orientation mapping. The obtained Kikuchi diffraction results demonstrate that the grain orientation in the polycrystalline nanowires is not simply random, but there is a texture induced by the shape of the former polymer nanowire in the green stage. Within an individual nanowire section, the dominating GBs are high-angle grain boundaries which play an important role in the current flow, e.g., in magnetoresistance experiments. Furthermore, the grain shape aspect of the LSMO grains is mostly elliptic, with the long axis oriented parallel to the outer edges of the nanowire

1D crystal geometry optimization using evolutionary computations

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Crystal structure prediction is a field of computational materials science which involve evolutionary algorithm approach combined with density functional theory to tackle a complex problem of finding the most favorable forms of condensed matter. In this work, we present current status of a custom general-purpose evolutionary algorithms library libbear [1], which we use for a problem of geometry optimization of 1D nanostripes. We provide detailed information about genetic algorithms methodology implemented in the library (genetic representation, variation operators etc.) as well as results of the 1D crystal geometry optimization calculations.

The prediction power of the libbear library combined with first-principles calculations will be tested by studying the structural, elastic, and electronic properties of atomic stripes made by group III and IV elements. A special focus will be placed on the investigation of the stability of the 1D structures against Peierls distortions. We obtain, for instance, that a zigzag boron stripe is so robust that does not undergo Peierls distortions at all. This is in contrast to aluminum stripes that are unstable with negative transverse phonon modes [2]. The transverse instabilities do not lead, however, to a gap opening. This is in clear contrast with the usual Peierls distortion picture that we observed, for instance, in carbyne [3]. We gratefully acknowledge support of National Science Centre under grant number UMO-2016/23/B/ST3/03575.

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Carbon monoxide and nitric oxide reaction on oxidized Al-Mo(110) surface alloy: A model prototype of noble-metal based heterogeneous catalysis

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One of the important aspects in modern heterogeneous catalysis is to find substitution of noble-metal based catalysts by those that do not consist of noble metals, but have the similar performance. One of the prototype reaction for noble metal catalysts (Rh, Pd, Pt and their alloys) is oxidation of carbon monoxide (CO) by nitric oxide (NO). In a search of non-precious metal containing substitutes, the present work focuses on study of coadsorption and interaction of CO and NO molecules on the Al-Mo(110) surface alloy and its oxide (Al-Mo-O). Investigations were carried out for corresponding model systems, in-situ formed in ultra-high vacuum, by a set of surface sensitive techniques. The Al-Mo(110) surface alloy was formed by annealing of several monolayer thick aluminium film deposited on the Mo(110) surface resulting in Al_2Mo stoichiometry with hexagonal surface atomic structure. Adsorption of CO molecules on the alloy surface with preliminary adsorbed NO molecules at a substrate temperature of 200 K dramatically affects the NO, displacing them to higher coordination sites with simultaneous tilting them to the surface plane. Annealing of this coadsorbed system to about 320 K results in CO oxidation by reduction of NO, much like the process realizing on noble metals. This effect is due to active surface sites appearing upon Al-Mo(110) alloying as well as to Mo d-band filling via sp-d hybridization. On the surface of the oxidized Al-Mo-O system obtained by holding the Al-Mo (110) system at a temperature of 700 K in an oxygen atmosphere to an exposure of 1500 L, the efficiency of the process of CO oxidation with nitric oxide significantly increases.

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Effect of plasmonic gold nanoparticles on collagen

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The electronic biosensor device plays an important and decisive role in medical conditions such as rheumatoid arthritis and the anti-glycation effect of collagen induced by gold nanoparticles. Tests for collagen and gold nanoparticles were performed on the biosensor electrical device and then characterizations were performed to identify the effect of anti-glycation of gold nanoparticles on collagen. The sample characteristics of the gold and collagen nanoparticles were done with SEM, EDAX, electrical testing and fluorescence optical spectroscopy. The gold nanoparticles have anti-glycation effect on collagen and elastin thus leading to the maintenance of collagen in good shape and avoiding glycation of collagen with sugars in the body which leads to breakdown of collagen and the appearance of skin wrinkles. AuNPs of 13 nm and 50 nm gold nanoparticles were prepared according to standard procedures, and their size was determined using SEM scanning electron microscopy. In the microchannel it is also mixed when applying the electric current of -5 and 5V then of -10 and 10V crosslinking and endogenous glycation and anti-glycation in the interaction with the gold nanoparticles occur. Investigating the analysis of our research has resulted in a good therapeutic effect of collagen with AuNP which have beneficial effect in rheumatoid arthritis and skin as well as in other conditions that have collagen deficiency. The basic mechanisms could be associated with the potential and anti-inflammatory of collagen in joints and AuNPs as antioxidant and anti-inflammatory. After investigating the efficacy of collagen with AuNPs, we recommend a novel therapeutic innovation in the treatment of anti-inflammatory and joint diseases. From the analysis of the collagen with AuNP with different concentrations and time durations are important to ensure that the therapeutic benefits are good medical effects.

Ab-initio theoretical calculations and experimental synthesis of $Sm_{1-x}MM_xCo_5$ (x = 0.1 – 1.0, MM = mischmetal)

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Permanent magnets are a key component for many technological applications for improving energy efficiency and addressing environmental and geopolitical issues. Sm–Co is the material of choice when high-temperature stability is required. $SmCo_5$ magnets exhibit high anisotropy ($\mu_0 Ha$ ~ 40 T), high Curie temperature (720 °C) and high energy product $(BH)_{max}$>150 kJ/m^3. Nevertheless, both Sm and Co need to be reduced or replaced by other elements due to cost, availability and environmental issues. Sm can be substituted by the mischmetal alloy (MM) which typically consists of cerium (Ce) and lanthanum (La). Ab initio atomistic simulations were used to determine the energetically favorable lattice sites in the P6/mmm hexagonal structure for the replacement of Sm atoms with the ones of the MM compound in the $Sm_{1-x}MM_xCo_5$ alloy for various stoichiometries. Furthermore, the impact of the distribution of MM atoms in the Sm lattice sites to the total and per atom magnetization for each configuration was important, as the energetically favorable configurations were different from the ones with the highest magnetization for fixed stoichiometry. $Sm_{1-x}MM_xCo_5$ configurations yielded a total magnetization as high as approximately 90% of the total magnetization of $SmCo_5$. A series of samples with nominal stoichiometry $Sm_{1-x}MM_xCo_5$ (x = 0.1 – 1.0) was prepared with Ar arc-melting and subsequent heat treatment. Annealed samples were studied with X-Ray diffraction and patterns show good crystallinity and small changes in unit cell parameters as expected. Curie temperature is reduced with increasing MM content almost linearly from 920 K (x = 0.1) to 800 K (x = 0.7) while in the case of the full-MM sample an enhanced Curie temperature is observed. Mass magnetization is not affected significantly across the series. It is deduced that the introduction of MM in $SmCo_5$ system may reduce the demand of Sm in some applications.

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WS3

P3-1 Novel manufacturing in producing nanofilters with enhanced properties against viral particles
V. Karagkiozaki, BL Nanobiomed P.C., Greece

P3-2 Extrusion-Based Cell-laden Gelatin/Alginate Hydrogel Bioprinting for Skin Tissue Engineering
Z.Chakim, BL Nanobiomed P.C., Greece

P3-3 Synthesis of polymer-coated silver nanoparticles for antimicrobial applications
L. Gkionis, BL Nanobiomed P.C., Greece

P3-4 Inclusion of Quercetin in Chitosan-capped Gold Nanoparticles. In vitro evaluation of their antioxidant and cytotoxic effect on human dermal fibroblasts
L. Gkionis, BL Nanobiomed P.C., Greece

P3-5 Quercetin PLGA nanoparticles against LPS induced inflammation in fibroblast cell lines
E. Papadopoulou, Aristotle University of Thessaloniki, Greece

P3-6 Polyvinyl alcohol (PVA) functionalized MgFe2O4 ferrite nanoparticles: encapsulation and release of doxorubicin for enhanced anticancer therapy
S. Mokhosi, University of KwaZulu-Natal, South Africa

P3-7 An Application of Multivariate Data Analysis to Photoacoustic Imaging for the Spectral Unmixing of Gold Nanorods in Biological Tissues
M. Maturi University of Bologna Italy

P3-8 Effects of silver nanoparticles on innate immunity in zebrafish and the protective effect of pterostilbene
Ying-Jan Wang, National Cheng Kung University, Taiwan

P3-9 Development and sterilization of a novel, modified, drug-eluting intraocular lens
Karamitsos A., 2nd University Ophthalmology Department, AUTh, Thessaloniki

P3-10 Identification and delivery of microRNAs that target the ribosomal machinery as a therapeutic strategy for hematological malignancies
Ioannis S. Vizirianakis, Aristotle University of Thessaloniki, Greece

P3-11 Synthesis and characterization of Chios Mastiha nanoparticles for biomedical applications (MASTIHA-NANO study)
Matthaios Didagelos, AHEPA University Hospital, Greece

P3-12 Synthesis of Mastiha based nanofibers for coating of angioplasty balloon
Ioakeim Giagtzidis, Aristotle University of Thessaloniki, Greece

P3-13 Stability of micron-sized cavitation nuclei within a therapeutic ultrasound field
Antonios N. Pouliopoulos, Columbia University, USA

P3-14 Engineering gold nanoparticle morphology for optimised microspectroscopic imaging of blood cancer cells
S. Boca, Babes-Bolyai University, Romania

P3-15 Modified with Curcumin PLGA nanoparticles in intranasal delivery of Galantamine adsorbed in novel Carbon Dots for Alzheimer's disease treatment
S.G. Nanaki, Aristotle University of Thessaloniki, Greece

P3-16 Leflunomide nanoparticles preparation via SBMA modified Chitosan
Stavroula G. Nanaki Aristotle University of Thessaloniki, Greece

P3-17 Simulation of waves of nonREM sleep
T.A. Vdovenkova, T.V.A. Canada

P3-18 Versatile mixed lipid monolayer shell and biodegradable polymer core Nanoparticles for biomedical applications
R. Cecchi NEST, Scuola Normale Superiore, Italy

P3-19 Study of synergistic antibacterial effects of silver nanoparticles combined with Vancomycin against E. faecium using fluorescence microscopy
L. Válková, Palacky University, Czech Republic

P3-20 Hybrid Nanoparticles for stimuli-triggered release of Tyrosine Kinase Inhibitors
Tatar A-S, Babes-Bolyai University, Romania

Novel manufacturing in producing nanofilters with enhanced properties against viral particles

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The COVID-19 presents a profound challenge for health systems, economies, but also the many gains that have been made in human health and global solidarity. The latest reports show that the virus has infected more than 7 million people worldwide with over 400.000 deaths. This situation demands for effective Personal Protective Equipment (PPE) for the protection of our health care workers and the general public. In this fight, Nanotechnology finds itself at the battlefront regarding the investigation of productive, cost effective solutions for our protection, considering that most of the commercially available masks are not eligible for the containment of this size of nanoparticles (SARS-CoV-2 dimensions are in the range of 50-140nm).
This study investigated the enhancement of fiber filters and their potential use in PPE. Samples of fiber filters were coated with a dispersion of polymer, creating nanoporous coatings, synthesized via chemical methods and deposited onto the fiber filters using Slot-die coating technique in order to produce nanofilters with high protection against the virus. We studied various concentrations and deposition parameters and their effect on the adhesion of the polymer material on the fiber filter. Our main goal was the reduction of the nanofilter's permeability and their further containment of the viral particles, approaching their dimensions. Finally, the morphology and structure of the nanofilters was characterized with Atomic Force Microscopy (AFM) and Optical Microscopy, and the permeability by filtration measurements. The results show that the permeability of nanofilters to nanoparticles was reduced to the desirable level, thus, the fabricated nanocomposite filters could be considered as effective alternative candidates to the current filter systems used in PPE.

Extrusion-Based Cell-laden Gelatin/Alginate Hydrogel Bioprinting for Skin Tissue Engineering

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3D Bioprinting is an emerging field in regenerative medicine utilizing 3D printing that combines cells and biomaterials to fabricate biomimetic structures. Current research on 3D printing technology for medical applications focuses on manufacturing biodegradable scaffolds and personalized tissue analogues, bringing new possibilities for building implants, pathological tissue models and alternative in vitro test methods. A crucial aspect of bioprinting is that he bioink must be biocompatible and have properties similar to the extracellular matrix (ECM) supporting cell adhesion and proliferation. In addition, bioinks used in extrusion bioprinting must have suitable rheological properties and crosslinking mechanisms, improving printability. Current skin bioprinting approaches mostly rely on the sequential printing of fibroblasts and keratinocytes embedded within a homogeneous hydrogel. Here, three Gelatin/Alginate hydrogel blends, by varying the individual constituent concentrations (6/5%, 6/7% and 6/9%), were investigated. Samples were tested for printability and viability of encapsulated L929 cells and NIH-3T3 cells (1.5×10^6, 3.5×10^6 and 7.5×10^6 cells) in bioprinted constructs. After 3D bioprinting and chemical cross-linking the constructs were stained 1, 4 and 7 days after incubation, using fluorescein diacetate (FDA) and Propidium Iodide (PI). The cross-linked bioprinted constructs retained their shape after 7 days. Also, high cell viability and changes in cell size and shape were observed. In conclusion, gelatin/alginate hydrogels have demonstrated good printability and biocompatibility.

Synthesis of polymer-coated silver nanoparticles for antimicrobial applications.

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The emerging field of nanotechnology covers a wide range of applications with biomedical and pharmaceutical fields to prevail among the others. Nanoparticles have been used as drug/gene delivery systems for the treatment of various pathologies for more than 30 years, owing to their unique properties such as their biocompatibility, enhanced aq. solubility, sustained drug release and tissue specificity, large surface area, small size and chemical versatility. Metallic nanoparticles derived from noble metals e.g. gold, silver and titanium, have recently gained increased interest not only for their ability to deliver therapeutics but also for their promising antimicrobial activity. Silver nanoparticles (AgNPs), specifically, have showed to exhibit significant antibacterial and antiviral activity in numerous studies, with a tolerant non-toxic concentration of 30 ppm in human cells.

In this study, we report the facile one-step synthesis of Ag NPs via reduction mechanism and the simultaneous coating with the anionic polymer polyvinylpyrrolidone (PVP). We investigated the stabilising effect of PVP over the size and size distribution of Ag NPs by varying the final polymer concentration. Different molar ratios of PVP content gave rise to nanoparticles ranging from 10 to 100 nm overall. All samples were characterized for their physicochemical properties by Atomic Force Microscopy (AFM) and Spectroscopic Ellipsometry respectively. Finally, the optimal in size nanoparticles (20-40 nm size range) were tested for their cytotoxic activity against the healthy murine skin fibroblasts (NIH-3T3) at different time points.

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Inclusion of Quercetin in Chitosan-capped Gold Nanoparticles. In vitro evaluation of their antioxidant and cytotoxic effect on human dermal fibroblasts.

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Nanotechnology has been largely implemented into pharmaceutical and cosmetical field for more than 20 years now. A variety of biocompatible nanocarriers including metallic nanoparticles, such as gold and titanium oxide, possess a range of demonstrated applications in cosmetology for the effective delivery of therapeutics into the upper skin layers. In particular, gold nanoparticles (Au NPs) are characterised by their non-toxic, highly stable and inert nature, their small size, the large surface area and crystallinity which altogether render them highly attractive and applicable for drug delivery purposes. Currently, Au NPs are being used in cosmetic industry in several products such as anti-ageing creams, deodorants and lotions. It has been reported that Au NPs can revitalise skin metabolism as providing advanced elasticity, skin firmness and anti-inflammatory plus antiseptic skin activity. Antioxidant molecules, with mainly phytochemical derived compounds, exhibit strong inhibitory free radical activity resulting in the prevention of biomolecules damaging and therefore mitigation of skin ageing process. The flavonoid quercetin is widely implemented in cosmetology for its anti-inflammatory and antioxidant activities. However, quercetin's poor aqueous solubility and low bioavailability limit its therapeutic efficiency. Nanocarriers come to bridge that gap upon the encapsulation of such lipophilic compounds.

In the current study, we report the development of small in size (10-20 nm size range), spherical and highly monodispersed Chitosan-capped Au NPs (CS-AuNPs) fabricated under mild acidic conditions, with the simultaneous conjugation of quercetin (CS-QAuNPs). Quercetin acted as the reducing agent of gold as well as the drug encapsulant. All samples were characterized for their physicochemical properties by Atomic Force Microscopy (AFM), UV-Vis spectroscopy and Spectroscopic Ellipsometry respectively. The CS-AuNPs and CS-QAuNPs, with an average size of 20 nm and 35 nm respectively, were tested for their cytotoxic and antioxidant activity against the healthy murine (NIH-3T3) and human (HaCat) skin fibroblasts.

Quercetin PLGA nanoparticles against LPS induced inflammation in fibroblast cell lines

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Abstract: Chronic inflammatory diseases are hard to treat and cause not only topical but also systemic symptoms. They are characterized by altered innate and acquired host immune responses and in general their etiopathogenesis is yet to be elucidated. Several chronic inflammatory diseases are not medically curable, although existing medications can alleviate and control the symptoms. In most cases a lifetime of anti-inflammatory drug therapy is necessary. For this reason, new drug delivery system development, preferably focusing on herbal substances with little to no adverse effects, is essential. Quercetin is a plant flavonoid known for its anti-oxidative and anti-inflammatory properties. However its bioavailability is generally poor due to low absorbance and rapid and extensive metabolism. Thus, a potent drug delivery system is required in order to make the most of quercetin's beneficiary effects against inflammation.
The aim of this study was to investigate the effects of quercetin encapsulated in PLGA nanoparticles, on the suppression of inflammation and the reinforcement of wound healing processes. To achieve this, inflammatory responses were induced in fibroblast cell lines (L929, NIH-3T3), using Escherichia coli lipopolysaccharide (LPS). The induction of wound healing environment, to simulate ulcers caused by chronic inflammatory diseases, for the assessment of the migration potential of the cells was achieved by wound healing assay. The PLGA nanoparticles were synthesized by nanoprecipitation and characterized by AFM. MTT assay and methylene blue staining were used to assess the cytotoxicity of the nanoparticles. The inflammatory response was measured, before and after the administration of the nanoparticle-encapsulated quercetin, by calculating the wound closure rate using optical microscopy and image analysis tools.

Polyvinyl alcohol (PVA) functionalized $MgFe_2O_4$ ferrite nanoparticles: encapsulation and release of doxorubicin for enhanced anticancer therapy

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Magneto-targeting presents as an intriguing method to enhance delivery of nanotherapeutics. Use of magnetic nanoparticles (MNPs) often entails their surface modification for tailored functional properties. To enhance biocompatibility and stability, MNPs are regularly conjugated with polymers such as chitosan, PEG and PVA. In this study, $MgFe_2O_4$ ferrite nanoparticles (NPs) were synthesized chemically via the glycol-thermal procedure. These were functionalised with the hydrophilic polymer polyvinyl alcohol (PVA) for the delivery of the anti-neoplastic chemotherapeutic drug, doxorubicin (DOX). The successful encapsulation of DOX onto PVA-$MgFe_2O_4$ NP surface was confirmed via fourier-transform infrared spectroscopy (FTIR). The shape, size and stability of the DOX-PVA-$MgFe_2O_4$ was examined using transmission electron microscopy (TEM) and nanoparticle tracking analysis (NTA). TEM revealed that the DOX encapsulated ferrite NPs possessed a quasi-spherical morphology with an average particle size of 17.65 nm. The DOX encapsulated ferrite NPs possessed a hydrodynamic size of 87.2 nm with a zeta potential of -25.2 mV, inferring an increased colloidal stability of the ferrite NPs. The drug encapsulation efficiency was 51.49% and release studies at pHs 4.5 - 7.4 over a 72 hour period showed a pH dependent release profile. Approximately 74.20% of DOX was released at tumor microenvironment pH 4.5 after 48 hours, and was sustained for 72 hours. The MTT and sulforhodamine B (SRB) *in vitro* cytotoxicity assays conducted on the human embryonic kidney (HEK293), the colorectal adenocarcinoma (Caco-2) and the breast adenocarcinoma (SKBR-3) cell lines demonstrated dose-dependent cytotoxicity profiles. The drug-nanoferrite complexes displayed increased specificity in the cancer cell lines, Caco-2 and SKBR-3, with cell viabilities of 38.72% and 35.56% obtained for the DOX-PVA-$MgFe_2O_4$ ferrite NPs at a concentration of 40 µg/ml. Dual acridine orange/ethidium bromide (AO/EB) staining showed that cell death occurred through both apoptosis and necrosis. To this end, DOX encapsulated PVA functionalized $MgFe_2O_4$ ferrite NPs may present as suitable candidates for magneto-targeted drug delivery.

An Application of Multivariate Data Analysis to Photoacoustic Imaging for the Spectral Unmixing of Gold Nanorods in Biological Tissues

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The increasing interest developing around photoacoustic (PA) imaging in the near infrared and its applications in tumour theranostics has directed great efforts of the scientific community towards the design of nanostructured contrast agents that could allow for active- or passive-targeted imaging of different regions of interest in vivo. However, multispectral imaging techniques often suffer from interferences from endogenous contrast and unambiguous identification of the sources of PA response is sometimes hard to perform. To overcome this issue, in various different multispectral imaging techniques, multivariate data analysis has represented a useful approach to generate images that can be related to a whole spectral profile, rather than be limited to the representation of the response at a single wavelength. In this work, we present an application of multivariate analysis (multivariate curve resolution – alternating least squares, MCR-ALS) to perform spectral unmixing in biological tissues in the presence of gold nanorods with various absorption properties.

Development and sterilization of a novel, modified, drug-eluting intraocular lens

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Purpose: Purpose: This study aims to assess the safety and the efficacy of two methods of development and of two methods of sterilization of a novel intraocular drug delivery system.
Setting/Venue: Lab for Thin Films - Nanobiomaterials - Nanosystems - Nanometrology, Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece
Methods: Spin-coating and spray-coating techniques were used , in order to develop polymeric, biodegradable, dexamethasone-eluting thin films on the surface of acrylic intraocular lenses. The same solution containing PLGA, PCL, Dexamethasone and chloroform as solvent was used in both techniques. Atomic Force Microscopy was contacted to characterize the surface of the modified lenses. Furthermore, the modified lenses were submitted to treatment with ultraviolet radiation for 20 minutes and H_2O_2 plasma sterilization, as per standard protocol. Imaging and in vitro cell culture studies were performed.
Results: Spin coating allowed development of thin films of uniform thickness over the desired area but spray-coating failed to cover the entire surface of the intraocular lens. Both sterilization techniques proved to be efficient in sterilizing the modified lenses. Plasma treatment caused cracks to the polymeric thin films, which was not noted with ultraviolet radiation.
Conclusions: Both sterilization techniques produce satisfactory results in terms of sterilization. Ultraviolet radiation does not affect the structure of the polymeric thin films.

Identification and delivery of microRNAs that target the ribosomal machinery as a therapeutic strategy for hematological malignancies

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Abstract: Ribosomes are the primary sites of protein synthesis within the cells of all domains of life. Due to this vital role in translation, ribosome numbers increase dramatically in cancer cells in order to support the vastly incremented metabolic needs required for cell multiplication. Therefore, the pharmacological interventions aimed at restoring ribosomal levels to their prior homeostatic condition have drawn great research and clinical interest, especially in ribosomopathies. The small non-coding RNA (miRNA) molecules emerge as targeted pharmacological nano-agents due to their repressive role in cellular processes. In this work, we hypothesized that miRNA molecules could be leveraged to target main ribosomal components, namely the ribosomal proteins, and thus being capable to restore the deregulated ribosomal function in hematological disorders. In order to identify candidate miRNAs, we performed a combined *in silico* and *in vitro* analysis, which revealed seven miRNAs, hsa-mir-16-5p, hsa-mir-92a-3p, hsa-mir-615-3p, hsa-mir-484, hsa-mir-100-5p, hsa-mir-186-5p, and hsa-mir-320a, with an ability to target approximately 67% of the total number of ribosomal proteins. We, then, bioinformatically analysed the main cellular processes affected by those miRNAs and identified various enriched biological pathways, including ribosome biogenesis, cell cycle, p53 signalling and cancer development. Furthermore, we experimentally studied miRNA regulation in cellular models of erythroleukemia, which revealed altered expression of multiple of the selected miRNAs. The selected miRNAs will be loaded on novel drug delivery platforms, such as a self-assembling peptide nanofiber hydrogel, in order to assess the potential anti-cancer role of the miRNAs in cellular models of leukaemia. In conclusion, the identified miRNAs demonstrate an inhibitory role in ribosome biogenesis, thereby their exogenous nano-delivery into cells represent a promising drug development strategy.

Synthesis and characterization of Chios Mastiha nanoparticles for biomedical applications (MASTIHA-NANO study).

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Introduction: Chios Mastiha (CM) is a natural resin with antioxidant, anti-inflammatory, anti-atheromatic, lipid- and glucose lowering properties.
Aim: To synthesize CM nanoparticles useful for possible biomedical applications.
Materials and Methods: CM powder was used to create PLGA-mastiha nanoparticles by the nanoprecipitation method. Characterization was accomplished by AFM microscopy.
Results: CM nanoparticles were synthesized, having a spherical appearance in AFM with a mean diameter of 148±41 nm (min=59 nm, max=216 nm) and a density of 1.7 x 10^9 Mastiha NP/ml.
Conclusions: This is the first study to synthesize CM nanoparticles. Nanoprecipitation is an effective method for this purpose. Analysis of the biological properties of CM nanoparticles with follow in order to assess their appropriateness for biomedical applications.

Synthesis of Mastiha based nanofibers for coating of angioplasty balloon

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INTRODUCTION: Atheromatosis and cardiovascular diseases are one of the leading causes of mortality globally. Endovascular intervention, and angioplasty with recently developed drug eluting balloons has evolved to be the cornerstone of treatment. Chios Mastic gum (CMG) is a natural resign with multiple properties including anti-inflammatory and anti-atheromatic. Drug delivery systems using nanotechnology is a relatively novel concept which offers multiple advantages and thus huge research and development is underway.**PURPOSE**: The purpose of the study was to develop drug eluting angioplasty balloons with CMG.**MATERIALS AND METHODS**: Polycaprolactone (PCL, molecular weight 70.000) with purified CMG powder diluted in chloroform was used in a syringe with 21G needle. Electrospraying was set at 30kV, with a volume of 10μl/min to synthetize mastiha based nanofibers using electrospraying method. Characterization was done with optical and AFM microscopy. A 5mm balloon for peripheral arteries was then used for electrospraying nanofibers under the same parameters and characterized with optical microscopy.**RESULTS**: PCL-mastiha nanofibers were synthesized with mean diameter of 460 nm and underwent cytotoxic study**.CONCLUSION**: This is the first study to synthetize CMG nanofibers and to use nanotechnology as carrier for drug eluting balloons. Further characterization for the nanofibers is pending. The efficacy of these angioplasty balloons will be studied and assessed with in vivo studies.

Stability of micron-sized cavitation nuclei within a therapeutic ultrasound field

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Microbubbles are micron-sized cavitation nuclei (diameter: 1-10 μm), which are routinely used in imaging and therapeutic ultrasound applications. Non-invasive and localized blood-brain barrier (BBB) opening using focused ultrasound (FUS) is an emerging therapeutic technique, which requires intravenous injection of pre-formed microbubbles. Although microbubble behavior during exposure to imaging sequences has been studied extensively, our understanding of microbubble stability within a therapeutic field is still incomplete. Here, we studied the temporal stability of microbubble cavitation activity during therapeutic FUS exposure in two timescales: the short time scale (i.e., μs of low-frequency ultrasound exposure) and the long time scale (i.e., days post-activation). Microbubbles flowing through a 4-mm vessel within a tissue-mimicking phantom (5% gelatin) were exposed to therapeutic pulses (f_c: 0.5 MHz, peak-negative pressure: 300 kPa, pulse length: 1 ms, pulse repetition frequency: 1 Hz, n=10). We recorded and analyzed the microbubble acoustic emissions with concentration-matched samples (10^7 microbubbles/ml) on day 0, 7, 14, and 21 after activation. Microbubbles had a concentration decay constant of 0.02 d^{-1} but maintained a stable size distribution for up to 3 weeks (< 10% variation). Temporal stability decreased while inertial cavitation increased over time both in vitro and in vivo, possibly due to changes in the lipid shell. BBB opening volume in mice (n = 3) measured through T1weighted contrast-enhanced MRI was equal to 19.1 ± 7.1 mm^3, 21.8 ± 14 mm^3, 29.3 ± 2.5 mm^3, and 38 ± 20.1 mm^3 on day 0, 7, 14, and 21, respectively, showing no significant difference over time (p-value: 0.49). In conclusion, micron-sized cavitation nuclei maintain their capacity to produce similar therapeutic effects over a period of 3 weeks after activation, as long as the natural concentration decay is accounted for.

Engineering gold nanoparticle morphology for optimised microspectroscopic imaging of blood cancer cells

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Abstract: Due to their unique size, shape, and environment-dependent physico-chemical properties, gold nanoparticles are emerging as novel contrast agents in various biomedical imaging techniques. This work focuses on investigating the impact of gold nanoparticle (GNP) morphology, and consequently of its plasmonic response, on the intracellular imaging capability by either dark field (DF) microscopy or surface-enhanced Raman scattering (SERS) spectroscopy. Starting from the basic sphere, various particle shapes including ellipsoids, triangles, hollow nanospheres and star-like were fabricated by one or two-step chemical synthesis route. Nile Blue (NB) cationic dye was used as model Raman reporter and SH-COOH heterofunctional PEG as particle stabilizer and ligand for the targeting antibody (Ab). The obtained AbGNPs complexes have good biostability and provide robust SERS signal under NIR (785 nm) excitation, which correlates with the plasmon resonance band of the solution-based nanoparticles. SERS imaging and DF microscopy on leukemia (CCRFSB-acute lymphoblastic leukemia) and lymphoma (SKW 6.4-human Epstein-Barr virus-transformed B cell) cells showed successful and preferential AbGNPs particle internalization by the targeted cells. The obtained results demonstrate that by controlling the particle morphology, we are able to obtain various AbGNPs compounds, with tunable optical properties and versatile conjugation surface for promising application in the identification and non-invasive microspectroscopic imaging of leukemia and lymphoma cells.

Acknowledgement: This work was supported by a grant of the Romanian National Authority for Scientific Research and Innovation, CNCS-UEFISCDI, project PN-III-P1-1.1-TE-2016-0919.

Modified with Curcumin PLGA nanoparticles in intranasal delivery of Galantamine adsorbed in novel Carbon Dots for Alzheimer's disease treatment

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PLGA-Curcumin was successfully synthesized, as showed by NMR, and characterized by FT-IR, XRD and DSC. The novel polymer was further used in nanoparticles preparation of galantamine, a drug used in Alzheimer disease. Furthermore, Carbon Dots (CDs), a novel carbon structure with small size spherical shape and good biocompatibility was used for encapsulation of high quantities of the drug. The resulting CD-Gal was also used in nanoparticles' preparation using as polymeric matrix PLGA-Curcumin. The two types of nanoparticles, net galantamine and adsorbed in CDs were characterized by DLS for their size, by FT-IR for possible bond formation, by XRD for their crystallinity and by DSC for their thermal properties. Net nanoparticles were also prepared for comparison reasons. Results showed that the particles formed was in the range of nanoscale while the drug was present in its amorphous form after its absorption in CDs. In vitro dissolution study was conducted in PBS at pH = 7.4. *In vivo* experiments are in process and will be conducted by intranasal administration in rat models.

This project has received funding from the Hellenic Foundation for Research and Innovation (HFRI) and the General Secretariat for Research and Technology (GSRT), under grant agreement No [1914].

Leflunomide nanoparticles preparation *via* SBMA modified Chitosan

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Psoriatic arthritis is a form of arthritis affecting patients suffering by psoriasis, a condition that features red patches of skin topped with silvery scales. Leflunomide is a common active pharmaceutical ingredient (API) used to treat such illnesses. Apart from its undesirable side effects (such as nausea, hair loss etc.) the drug is characterized by low aqueous solubility and restricted oral bioavailability. Hence, the utilization of new formulation approaches, based on nanoparticles, and alternative roots of administration (such as skin delivery) would be beneficial.
Chitosan (CS) is a linear, biocompatible polysaccharide used in several biomedical nano-based applications. In the present work, SBMA modified CS (CS-SBMA) was evaluated for the preparation of Leflunomide nanoparticles focusing on skin delivery. SBMA (which is a zwitterionic molecule) was selected for its antibacterial properties which are expected to lead to a further protection of affected skin area. The synthesis of the newly synthesized CS-SBMA nano-carriers was characterized by NMR and FT-IR, while its physical state and thermal properties were evaluated *via* XRD and DSC, respectively. Solubility in different pH and swelling studies were also conducted. The optimum CS-SBMA carrier was used for the nano-encapsulation of Leflunomide *via* ionic gelation. Drug-loaded nanoparticles were characterized by FT-IR, XRD and DSC, while their size was determined by DLS and compared to neat (blank) CS nanoparticles. *In vitro* dissolution studies were also conducted in PBS at pH = 7.4.
Acknowledgment: The proper study was co-funded by Greece and the European Union through action Human Resources Development, Education and Lifelong Learning (**EDBM 103, MIS: 5047916**).

Simulation of waves of nonREM sleep

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Being supposed basis for nanoengineering in memory improvement, nonREM IVth stage Slow Oscillations (SO) simulation from PFC neuron due to presynaptic VGCCs activation at cytosolic Na^+ ions accumulation at axon terminal by emitted electric field (**E**) during linear oscillation of electric charge $Q_{st\ min} = 4^x10^{-7}$ C at 0.75 Hz and 1 m distance is sensitive to cytosol relative permittivity (ε_r). At $\varepsilon_r = 3.84^x10^5$, SO are initiated in PFC neuron post-synaptic to PFC neuron with 2.5 mm projection of axon along **E** in 27.3 min [1].
In the present work, it is proposed that ε_r could be estimated from SANS activation [2] at simulation of nonREM IInd stage σ-waves in DG and/or CA1 neurons due to linear oscillation of electric charge $Q_{st\ max} = 35^x10^{-7}$ C at 7 Hz and 0.1 m distance along axons of ER neurons. Calculation has shown that for SANS activation at the 3rd linear oscillation along ER neuron axon with 15 mm projection along **E**, ε_r are $7.5^x10^4 \div 9.2^x10^4$. For these ε_r, SO are initiated from the PFC neuron due to linear oscillation of electric charge $Q_{st\ min} = 4^x10^{-7}$ C at 0.75 Hz and 1 m distance in 1.04 ÷ 1.58 min. This time is overestimation for shorter projection of ER neuron axon along **E**.
[1] Vdovenkova T.A., Simulation of waves of deep sleep, Symposium “Bioinspired and biointegrated materials as new frontiers nanomaterials VIII”, 17 - 20 September, 2018, Warsaw, Poland.
[2] Vdovenkova T.A., Private view on circadian rhythms of brain activity, Symposium “Bioinspired and biointegrated materials as new frontiers nanomaterials VII”, 22 – 26 May, 2017, Strasbourg, France.

Versatile mixed lipid monolayer shell and biodegradable polymer core Nanoparticles for biomedical applications

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Abstract: Potential benefits of drug delivery via nanoparticles led to the creation of a huge variety of these nanoconstructs. We optimized an easily customizable type of nanoparticles (NPs), consisting of a lipophilic core containing a biodegradable polymer coated by a lipid monolayer. We assessed that our kind of NPs is obtainable by different methods (nanoprecipitation, emulsion, double-emulsion).
In order to follow the fate of these NPs upon internalization by living cells via confocal fluorescence microscopy, we fluorescently labelled both the main components, and eventually also loaded drug mimicking fluorophores in the core; however, these nanoparticles can be easily labelled with other kinds of tracers with the aim to locate them in tissues or even living organisms (e.g. by NMR imaging, photoacoustic, possibly PET).
With specific protocols we tried to enhance the encapsulation of a water poorly-soluble drug (Pioglitazone) and a lightly soluble one (Methotrexate, logP=-1.85), in order to obtain stable nanoparticles with a satisfactory encapsulation efficiency.
The first cell models we are considering are immune cells, since they are among the first interacting species found by NPs upon injection in an organism. In particular, monocytes models are considered, also after their transformation into foam cells.
These specific drugs and cell models were chosen for their relation to cardiovascular diseases studies, *e.g.* atherosclerosis ones. I shall present our original results, discussing the main advantages and possible complications in the synthesis technique, and its possible biomedical applications.

Study of synergistic antibacterial effects of silver nanoparticles combined with Vancomycin against *E. faecium* using fluorescence microscopy

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Silver nanoparticles (NPs) strongly enhance antibacterial activity against broad spectrum of bacterial strains when combined with antibiotics. However, the mechanism of their synergistic effect is not yet fully understood and may vary for different bacterial strains and antibiotics. In this work we present a mechanism of the combined antibacterial effect of silver NPs and Vancomycin against *E. faecium* strain sensitive and resistant to Vancomycin. For the first time the synergistic mechanism was described based on the localization of fluorescent labeled silver NPs and Vancomycin BODIPY FL fluorescent conjugate using high resolution fluorescence microscopy. It can be concluded that the synergistic effects of silver NPs and Vancomycin mainly consists in the mutual disruption of the permeability and strength of the cell wall, which becomes unstable and loses its strength and it is subsequently disrupted and detached. In addition, silver NPs significantly deform bacterial DNA, which also significantly contributes to the inhibition of bacterial growth. This work can help to better understand the mechanisms of synergistic effects of silver NPs with antibiotics against resistant bacteria which represent an important finding for potential approach to an effective fight against the unresolved problem of an increasing resistance of pathogenic bacteria against traditional antibiotics. The authors gratefully acknowledge the support provided by the project No. 19-22720S of the Czech Science Foundation.

Hybrid Nanoparticles for stimuli-triggered release of Tyrosine Kinase Inhibitors

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Abstract: With cancer being among the leading causes of death globally, nanomedicine is undertaking intense efforts to fight the disease. Various challenges can be addressed *via* nanotechnology, which may offer advantages such as improved and triggered drug release, active targeting, or competitive molecular inhibition, and can be combined with applications like cellular imaging. A class of highly promising anti-cancer drugs are Tyrosine Kinase Inhibitors (TKIs), small molecules that specifically inhibit the activity of kinases involved in cancer proliferation. Although superior to chemotherapeutics, the hydrophobicity and low bioavailability of TKIs require further and constant development of new formulations.

Herein we aim to develop hybrid nanoparticles with a plasmonic core and an amphiphilic pH-responsive polymeric shell as carriers for the anti-leukemic TKI Midostaurin. The optimisation of the organic layer is based on either Pluronic-F127, Polyvinylpyrrolidone-(PVP) or Poly(2-(dimethylamino)ethylmethacrylate)-(PDMAEMA) polymers that offer hydrophobic pockets for drug-loading, a hydrophilic corona for improved solubility, and the added pH-sensitivity for controlled-release. Drug-loading and pH-controlled release in acidic buffer solutions were investigated using UV-Vis-NIR absorption and fluorescence spectroscopy. Further on, the nanoparticles are amenable to antibody functionalization for specific targeting of the leukemic cells.

By ensuring efficient delivery at the diseased site and reduced systemic side-effects, the proposed hybrid nanoparticles have the potential to improve the treatment efficiency of TKI drugs.

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WS4

P4-1 Culture-independent detection of carbapenemase-producing bacteria with plasmonic nanosensors
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P4-2 Nanoparticle Reservoirs for Paper Inmunosensors
Alejandra Alba-Patiño Son Espases University Hospital, Spain

P4-3 Synthesis, Characterization, and Sintering Behavior of Doped Nanocrystalline Ceria Powders
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P4-4 Flexible sensing solutions for healthcare and biotechnological applications
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Culture-independent detection of carbapenemase-producing bacteria with plasmonic nanosensors

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Abstract: Sepsis is an overwhelming reaction to an infection leading to organ dysfunction, which can cause death in a few hours. Therefore, it is essential to provide the right antibiotic treatment as soon as possible in order to improve patients outcomes1. The treatment usually consists of administering broad-spectrum antibiotics, such as carbapenems. However, various microorganisms have developed different methods to protect themselves against these antibiotic-based therapies. For example, many bacteria produce carbapenemases, a wide family of enzymes which can hydrolize the scaffold of β-lactam antibiotics with a high catalytic efficiency2. Here a new diagnostic method is reported for detecting βlactamase-producing bacteria without longsome culture procedures. It consists of aggregating gold nanoparticles as a function of the pH variation caused by the specific hydrolisis of the antibiotic, giving a color change visible to the naked eye. The method proposed here can detect carbapenemase-producing bacteria above the infectious threshold within a few hours and at the point of care, even when these bacteria are mixed with a large excess of non-resistant pathogens. The system was validated with a panel of urine and sputum samples, obtained from a large cohort of patients. The nanosensors provide rapid information with a decentralized detection scheme that can be applied by the bedside, and therefore could be used to personalize the antibiotic treatment in the context of sepsis.

1 Journal of Antimicrobial Chemotherapy 2017;72:2519-2527
2 NewJ.Chem. 2016;40(3):1982–1987

Nanoparticle Reservoirs for Paper Inmunosensors

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Abstract: Paper-based biosensors or paper analytical devices are increasing their popularity in all fields because of their low cost, easy fabrication, and portability. Utilizing paper as a substrate presents several advantages such as biodegradability, disposability, biocompatibility, storing of reagents and liquid flowing by capillarity. These features permit the operation of the device without the need for any additional equipment 1.
Gold nanoparticles (AuNPs) have been widely used as probes for colorimetric signal transduction due to their strong color, high extinction coefficient and easy functionalization with a biological recognition element (protein, antibody, enzymes, etc.)1. However, it is difficult to store them reversibly in paper substrates because once they dry they cannot be removed from the cellulose matrix. Therefore, it is critical to find a method for integrating these nanoprobes in cellulose matrices to obtain biosensors made entirely of paper1.
In this work, we propose a new method to store protein-decorated AuNPs in filter paper that also allows releasing them when required. This AuNPs reservoir is made by means of modifying the filter paper with polystyrene sulfonate (30%). Nanoparticles deposited in the modified paper can be transferred to a receiving wet paper containing the analyte with high efficiency. To test this method, we integrated this reservoir in a paper biosensor for the detection of glycoprotein B from human cytomegalovirus in serum samples, obtaining a low limit of detection of 0.03 ng·mL-1 with a total assay time of only 12 minutes. The densitometric measurement performed in this approach could also be made by smartphone with an augmented reality app developed in our lab2, making the proposed paper-only biosensors ideal for point-of-care diagnostics.
1ACS Sensors. 2020;5:147–53. 2 Nanoscale Adv. 2020;Available: http://dx.doi.org/10.1039/D0NA00026D.

Synthesis, Characterization, and Sintering Behavior of Doped Nanocrystalline Ceria Powders

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Cerium oxide (CeO2) is one of good candidates for the high performance gas sensors, it is a single phase oxide with high homogeneity region, which show some promising features for application as a sensors . It was shown that dopped nanosize ceria exibits a good results for selective detection of ppm-level of H2S and NO2 [1]. Short response time, relatively low working temperature of oxygen gas sensors was shown in [2] for porous ittria doped CeO2 structure which was sintered from nanosize powder. In the recent study, the nanocrystalline CeO_2 powders doped by different rare earth metals have been successfully synthesized by a chemical precipitation from cerium nitrate (III) by formation of cerium pseudo-alcoholates with their subsequent oxidation to cerium (IV) oxide. It was shown that cerium oxide is formed during the synthesis process and the resulting powder does not require high-temperature heat treatment. The size distribution of the resulting particles, and the average particle size as a function if synthesis parameters had been studied. The effect of the drying temperature of the powder on the average particle size is shown. The kinetics of sintering of the obtained nanopowder was studied; it was shown that sintering at a temperature of 1100 degrees Celsius makes it possible to obtain ceramic samples with a density of 92-96% with mesoporous structure. The resulting material is promising for use as low-temperature oxygen sensors.
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[2] D. W. Lee, et al. // Mater. Sci. Forum. 534-536 (2007) 61-64

Flexible sensing solutions for healthcare and biotechnological applications

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In the last years, several applications have been envisaged for printed electronics, being the biotechnology area one of the major focus. From low-cost and flexible smart devices, a substantial number of printed devices is already in the market or in an upscaling and industrialization processes. Herein, we show a novel solution based on the development of flexible printed devices to monitor a wide range of biotechnological processes and the degree to which a patient correctly follows medical advice. In the first case, the co-operation with automation systems solution intends to achieve a more accurate observation and control of the biotechnological industry processes, particularly in chromatography techniques and high-throughput downstream purification processes. In partnership with Portuguese companies, Neutroplast and Beyondevices, and Turkish companies, Turgut and Robotek, CeNTI, a Portuguese research Centre, is developing and integrating flexible printed sensors into microwell plates and medicine bottles, to monitor a wide range of volume solutions. Additionally, novel printed sensors are being developed and integrated into falcon tubes to monitor other parameters such as pH and ionic conductivity in biotechnological downstream processes. In this case, printed electronics plays a crucial role, allowing a substantial reduction of costs, weight and thickness while being disposable. Recent developments on production and integration of flexible sensors, with a minimal volume sensitivity of 40μl, and additional parameters such as pH, and ionic conductivity will be presented.
This work was developed in the scope of European project SR4SB and national project DOSEA (n. 33664), which was co-financed by Portugal 2020, under the Operational Program for Competitiveness and Internationalization (COMPETE 2020) through the European Regional Development Fund (ERDF).

WS5

P5-1 Theoretical prediction of Sb2Se3 growth morphology and orientation on muscovite mica substrates
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P5-2 Influence of intrinsic vacancies on the photocatalytic properties of hybrid ZnS/WS2 nanotubes: Prediction from first principles
I. Isakovica, University of Latvia, Latvia

P5-3 CO2 electroreduction toward C2H4 at Cu decorated graphene nanofilm: Prediction from first principles
S. Piskunov, University of Latvia, Latvia

P5-4 Investigation of graphene based resistive strain sensors for vital signal monitoring
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P5-5 Conductive Smart-Inks development base on Graphene and MoS2 and their uses in Ink-Jet systems
J. Rubio, Universidad Central

P5-6 Investigation of treatment parameters on electrical properties of graphene
E.S. Vasilyeva, Saint Petersburg Polytechnic University Russia

Theoretical Prediction Of Sb_2Se_3 Growth Morphology And Orientation On Muscovite Mica Substrates

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Ever since the first demonstration, van der Waals (vdW) heterostructures have received considerable attention due to their unique interlayer coupling and optoelectronic properties. Sb_2Se_3 is a quasi-one-dimensional material that can form vdW heterostructures on other low dimensional or 3D substrates and has shown excellent optoelectronic properties. However, despite few experimental works, the growth mechanism of Sb_2Se_3 on low dimensional substrates is elusive. Under equilibrium conditions, the growth of low dimensional materials is governed by vdW epitaxy. As in classical epitaxy, the growing layer adopts specific orientation to minimize lattice mismatch. The structure of Sb_2Se_3 resembles that of the molecular crystal, therefore the epitaxial relationship on the specific substrate can be estimated through relatively simple algorithm. In this work, we aim to predict the orientation of low dimensional materials grown on the specific substrate.
As a case study, we chose to examine epitaxial relation of Sb_2Se_3 and muscovite mica. The determination of the optimum overlayer orientation was accomplished using a simple geometric lattice misfit modelling algorithm that calculates a "dimensionless potential". Out of 10 tested planes with miller indices of (hk0), where h varied in 1 to 3 and k in 1 to 5 range, the (120) indicated the point-on-line coincidence at azimuthal angle at θ~90 and 270 deg. A fair agreement was found with experimental results available in the literature. The existence of lattice coincidence verify that molecular crystal lattice misfit modelling algorithm can be suitable for prediction of Sb_2Se_3 morphology and orientation, and could be helpful in vdW epitaxial growth of 1D/2D p-n heterostructures optimization and selection of the substrates.

Influence of intrinsic vacancies on the photocatalytic properties of hybrid ZnS/WS_2 nanotubes: Prediction from first principles

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Abstract: Engineering the electronic energy band structure of hybrid nanostructured semiconductor materials through judicious control of their atomic composition is a promising route to increase visible light photoresponse, which is necessary prerequisite for many photocatalytic processes, e.g. photocatalytic water splitting to H_2 and O_2. In this study we have carried out the first principle calculations to simulate the electronic structure of hybrid ZnS/WS_2 nanotubes containing intrinsic sulphur vacancies. Ab initio modelling reported here have been performed within the formalism of hybrid Density Functional Theory and Hartree-Fock method using HSE06 exchange-correlation functional, which is properly adapted and verified relatively to properties of ZnS and WS_2 bulk and nanosheets. Pristine ZnS/WS_2 nanotubes has been predicted to be attractive for photocatalytic water splitting under influence of solar light. The defect induced levels at the band gap of ZnS/WS_2 nanotube containing sulphur vacancy are properly aligned relative to the oxidation and reduction potentials necessary for water splitting under visible light irradiation. The edges of band gap of defective ZnS/WS_2 nanotube correspond to the range of visible spectrum. Funding from Latvian Council of Science fundamental and applied research project Nr. LZP-2018/2-0083 is greatly acknowledged.

CO_2 electroreduction toward C_2H_4 at Cu decorated graphene nanofilm: Prediction from first principles

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Abstract: The electrochemical reduction of CO_2 is a promising green approach to convert CO_2 into usable form of carbons. The monodisperse Cu nanoparticles assembled on a single layered graphene can support mass- and size-dependent catalysis for the selective electrochemical reduction of CO_2 to ethylene (C_2H_4). The properly treated (e.g. N-doped) graphene itself can catalyse the CO_2 reduction to formate, but the composite graphene-Cu structure functions as a CO_2 and proton absorber, facilitating hydrogenation and carbon–carbon coupling reactions on Cu-nanocluster for the formation of C_2H_4. In this study, we employ density functional theory calculations to examine different active sites in Cu-decorated graphene, to give an outline of the trends in its catalytic activity. We found that adsorption energies of CO_2 and CH_2 do not follow the linear scaling relationships observed for the pure transition metals, and this unique scaling is rationalized through differences in electronic structure between transition metals and graphene. This finding rationalizes most of the experimental observations on the carbon-based materials which present promising catalysts for the two-electron reduction of CO_2 to CO. With thermodynamic analysis, we identify active sites that are expected to exhibit a comparable or even better activity to the state-of-the-art copper catalysts, and the best configurations are suggested to be selective for CO_2 reduction reaction. Funding from European Union`s Horizon 2020 Research and Innovation Program project under grant agreement No 768789 is greatly acknowledged.

Investigation of graphene based resistive strain sensors for vital signal monitoring

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Abstract:

The growing interest in wearable devices for personalized health monitoring, human motion detection, soft robotics and so forth has led to a rapid development of flexible strain sensors over the last few years. Most of them use nanocomposites as sensitive layers and elastomeric materials as low cost substrates that can be easily processed. Carbon based nanocomposites, such as graphene, have prevailed over other nanomaterials due to their superior properties, low cost and high flexibility in terms of their processing. In this work, we fabricated resistive strain sensors using graphene encapsulated in a polydimethylsiloxane PDMS matrix (sylgard 184).

The sensors have 2 cm length and 1 cm width and have been fabricated with a simple method based on drop-casting of both PDMS and a graphene dispersion. In order to test their feasibility for vital signal monitoring, the sensors were tested under static and dynamic load for small strain values using a cantilever beam setup. We also evaluated the effect of parameters such as temperature, contacts and material properties (such as base:curing agent ratio for the PDMS, and dispersion properties for graphene).

The resistance of the sensors is in the range of a few KOhms and the gauge factor is about 25 at 0.2% strain. Base:curing agent ratio of 10:1 is superior to 30:1 in terms of temperature drift and hysteresis, although the elastic modulus of 30:1 ratio is closer to that of the human skin and may present better adhesive properties. The best yield and sensor stability was obtained for sensors with copper tape in combination to silver paste as contact materials.

Conductive Smart-Inks development base on Graphene and MoS_2 and their uses in Ink-Jet systems

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This Smart INK project is based on the study of carbon-based nanomaterials, mainly the use of graphene and MoS_2 as active agents in the design of electrically conductive inks, which allow to write, draw or print circuits in a simple way, intuitive, fast and effective. As an innovative project, since there are no active nanoparticle-based inks on the market, Smart INK had an important research phase. This study shows the progress of the research along with some of the tests carried out in the scanning electron microscope SEM-EDS, specifying the technical processes used and the main results achieved. One of the most relevant findings of the research were the low levels of electrical resistance obtained (26 – 80 □□sqr) using ink on a cellulose polymer substrate. It was also shown that ink retains its properties over time and after hundredths stress cycles.

Investigation of treatment parameters on electrical properties of graphene

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Graphene is an allotropic two-dimensional carbon modification with a hexagonal crystalline structure. Graphene is used in many fields of electronics: from transistors to biochemical sensors and OLED diodes (organic light emitting diodes) due to its unique properties such as high carrier mobility (above $2 \cdot 10^5$ $cm^2 \cdot B^{-1} \cdot c^{-1}$). There are various types of processing to obtain the graphene samples with the certain parameters needed for further application: alloying, intercalation, irradiation or annealing. In order to use graphene as a material for flexible electronics, for example, as a nanocomposite filler, there is no point in intercallation, and impurity deposition only changes the type of conductivity or increases its resistance.
Therefore, annealing was used as a method of modifying the properties of graphene. In this work the influence of an additional annealing of graphene on its electrical properties was studied for two different regimes (250 °C and 400 °C). We found that an additional graphene annealing modifies the slope of the temperature dependence of the resistance and its value. Annealing at 400 °C increases the resistance value, and at 250 °C- decreases. In addition, the slope of the dependence changes more in the sample annealed at 400 °C. It means, that the annealing of graphene consists of two processes: cleaning of the graphene surface and defect formation. The annealing at relatively high temperatures is more often accompanied by the defects' formation, but the change in the slope of the dependence indicates the cleaning of the sample surface. Changes in carrier mobility of graphene in polymer film under different concentration and percolation rate experimentally and theoretically studied in this work. Flexible composite with deformation rate depending conductivity can be successfully applied as a substrate for flexible electronic devices, sensors and smart textile.

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